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SYNTHESIS OF CUBANE BASED ENERGETIC MOLECULES

October 1988

Annual Report

By:

Robert J. Schmitt and Jeffrey C. Bottaro
Energetic Materials Program

Prepared for :

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The objective of this research is to develop new methods for the functionalization of the cubane nucleus and to synthesize energetic cubanes for use as high energy propellants, explosives, or both. Recent achievements in this program include sutdies on new methods of cubane functionalization that have resulted in a considerably more efficient method for the synthesis of the important intermediate cubane-1,2,4,7-tetracarboxylic acid and an improved procedure for the synthesis of 1,4-cubane diol. We have also done the first preparation of several energetic polynitrocubanes: cubane-1,2,4,7-tetrakis(β,β-dinitro-β-fluoroethylester), cubane-1,4-bis(β,β,β-trinitroethylester), cubane-1,2,4,7-tetrakis(β,β,β-trinitroethylester), N,N'-bis(β,β-dinitro-β-fluoroethyl)-1,4-diaminocubane, N-nitro-N'-nitroso-bis-N,N'-(β,β-dinitro-β-fluoroethyl)-1,4-diaminocubane, and N,N'-dinitro-bis-N,N'-(β,β-dinitro-β-fluoroethyl)-1,4-diaminocubane. The highly energetic 1,4-dicyanocubane and cubane-1,4-diisocyanide have been synthesized. We are now attempting to synthesize cubane-1,4-dinitrate and other more highly nitrated cubanes as well as the energetic fuel 1,2,4,7-tetracyanocubane.

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Senior Vice President
Sciences Group

A-1

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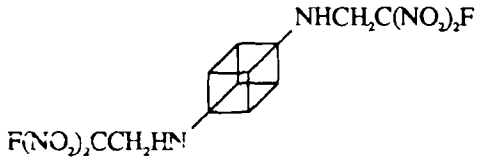
SUMMARY

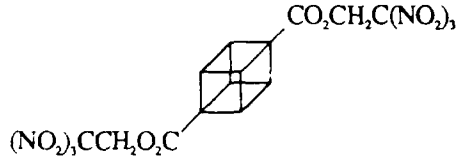
The objective of this research is to develop new methods for the functionalization of the cubane nucleus and to synthesize energetic cubanes for use as high energy propellants, explosives, or both. Recent achievements in this program include studies on new methods of cubane functionalization that have resulted in a considerably more efficient method for the synthesis of the important intermediate cubane-1,2,4,7-tetracarboxylic acid and an improved procedure for the synthesis of 1,4-cubane diol. We have also done the first preparation of several energetic polynitrocubanes: cubane-1,2,4,7-tetrakis(ß,ß-dinitro-ß-fluoroethylester), cubane-1,4-bis(ß,ß,ß-trinitroethylester), cubane-1,2,4,7-tetrakis(ß,ß,ß-trinitroethylester), N,N'-bis-(ß,ß-dinitro-ß-fluoroethyl)-1,4-diaminocubane, N-nitro-N'-nitroso-bis-N,N'-(ß,ß-dinitro-ß-fluoroethyl)-1,4-diaminocubane, and N,N'-dinitro-bis-N,N'-(ß,ß-dinitro-ß-fluoroethyl)-1,4-diaminocubane. The highly energetic 1,4-dicyano-cubane and cubane-1,4-diisocyanide have been synthesized. We are now atttempting to synthesize cubane-1,4-dinitrate, and other more highly nitrated cubanes as well as the energetic fuel 1,2,4,7-tetracyanocubane.

The following five pages summarize the energetic cubanes synthesized thus far, our plans and projected progress for year 3, and our long term goals and plans for this project.

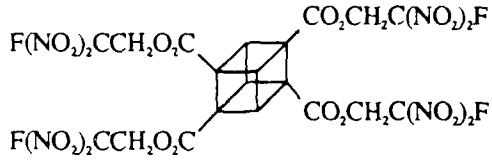
Energetic Cubanes Synthesized



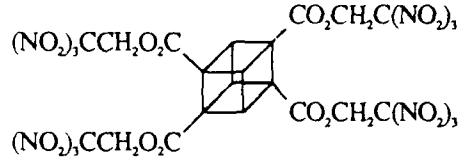
July 1986. N,N'-Bis-N,N'-(ß,ß-dinitro-ß-fluoroethyl)-1,4-diaminocubane. The first energetic cubane derivative, precursor to other, more energetic cubanes.



January 1987. Cubane-1,4-bis-(ß,ß,ß-trinitroethylester). Model for other, more highly functionalized energetic cubyl esters.



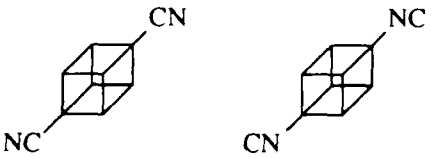
October 1987. Cubane-1,2,4,7-tetrakis(ß,ß-dinitro-ß-fluoroethylester). The first fully oxidized cubane.



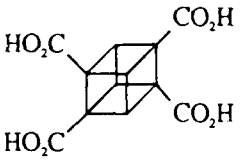
October, 1987 Cubane-1,2,4,7-tetrakis(ß,ß,ß-trinitroethylester). The first overoxidized cubane derivative.

Energetic Cubanes Synthesized

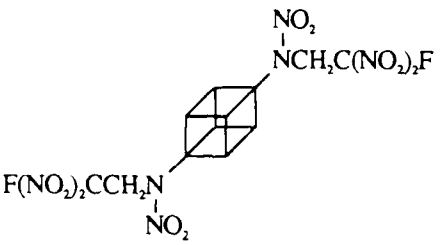
-Concluded-



January 1987. 1,4-Dicyanocubane. April 1988. 1,4-Diisocyanocubane. First examples of new cubane fuels using cyano and isocyano groups to increase the heat of formation. Calculated heat of formation +191 kcal/mol and +221 kcal/mol respectively.



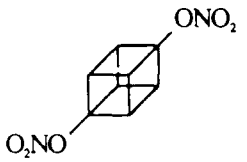
July 1988. Cubane-1,2,4,7-tetraacid. New, shorter, and more efficient synthesis of this important intermediate.



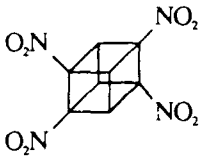
August 1988. N,N'-Dinitro-bis-N,N'-(ß,ß-dinitro-ß-fluoroethyl)-1,4-diaminocubane. Model compound for the tetrasubstituted derivative.

Plans and Projected Progress for Year 3

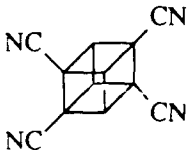
Synthesis of the Following Target Compounds:



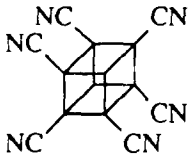
Complete the synthesis of cubane-1,4-dinitrate. A more highly oxidized cubane derivative.



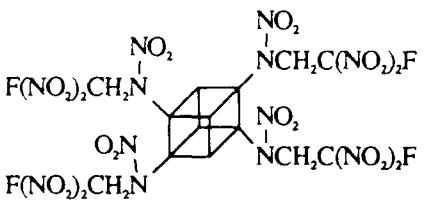
1,2,4,7-Tetranitrocubane. The next energetic cubane.



1,2,4,7-Tetracyanocubane. Cubane based fuel with a calculated heat of formation of +253 kcal/mol.



1,2,3,4,6,7-Hexacyanocubane. Cubane based fuel with a calculated heat of formation of +314 kcal/mol.



Tetrakis-1,2,4,7-(N-nitro-ß,ß-dinitro-ß-fluoroethylamino)cubane. Overoxidized, highly energetic oxidizer.

Plans and Projected Progress for Year 3

-Concluded-

Investigate New Synthetic Methods and Other Energetic Cubanes

- Study photochemically catalyzed nitrations of cubanes
- Develop new oxidations of protected cubylamines to give polynitrocubanes
- Synthesize polycyanocubane and polyisocyanocubanes as fuels
- Synthesize cubylperchlorates
- Improve efficiencies and yields in all steps.

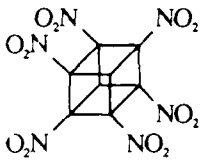
Long Term Goals and Plans

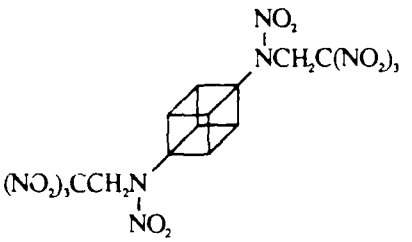
Goal: Develop new methods for the synthesis of energetic cubanes and synthesize new energetic cubane derivatives.

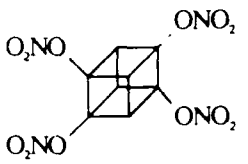
Approach: Further exploit the chemistry being developed for the cubane nucleus to synthesize compounds with high density and high positive heat of reaction.

Targets:

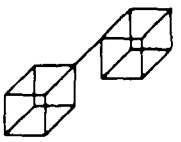
- Synthesize more highly nitrated cubanes



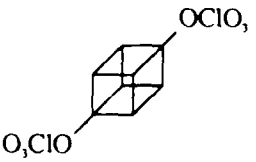


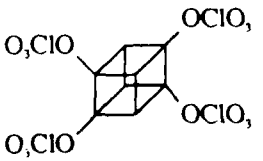


- Synthesize propellants based on cubyl-cubane



- Synthesize cubylperchlorates





- Develop new routes to the cubane nucleus
- Improve the efficiencies of all steps
- Develop new methods for nitro group introduction into the cubyl nucleus.

INTRODUCTION

The need to pack more power with less weight into less space in tomorrow's weapons drives this program for the synthesis of new generations of superenergetic materials based on cubane. Cubane's heat of formation (+149 kcal/mol), density (1.29 g/cm^3), and strain energy (+166 kcal/mol) are extraordinarily high, a combination not exceeded by any other stable hydrocarbon available in reasonable quantities. The addition of groups that are energy-rich, oxidizing, or both will create exceptionally dense and powerful explosives, propellants, and fuels. For example, calculations predict that octanitrocubane will be a radical improvement over currently available explosive materials; present estimates put it 25% better than HMX.

The cubane system is geometrically very different from ordinary compounds and thus requires the development of innovative methods to prepare substituted cubanes. To do this in sensible ways requires a keen appreciation of the effects of distorted geometry on reactivity, the subject of much speculation and hypothesis for the past two decades. This SDI/IST project provides for the first time extended testing of the theories of organic chemistry regarding highly strained compounds. We have already made considerable progress turning theory into practice. Novel methodology has been developed for the systematic substitutions and functional group transformations on the cubane nucleus. The first energetic cubanes have been synthesized, including the only cubanes that are sufficiently oxidized to be considered as propellants or explosives.

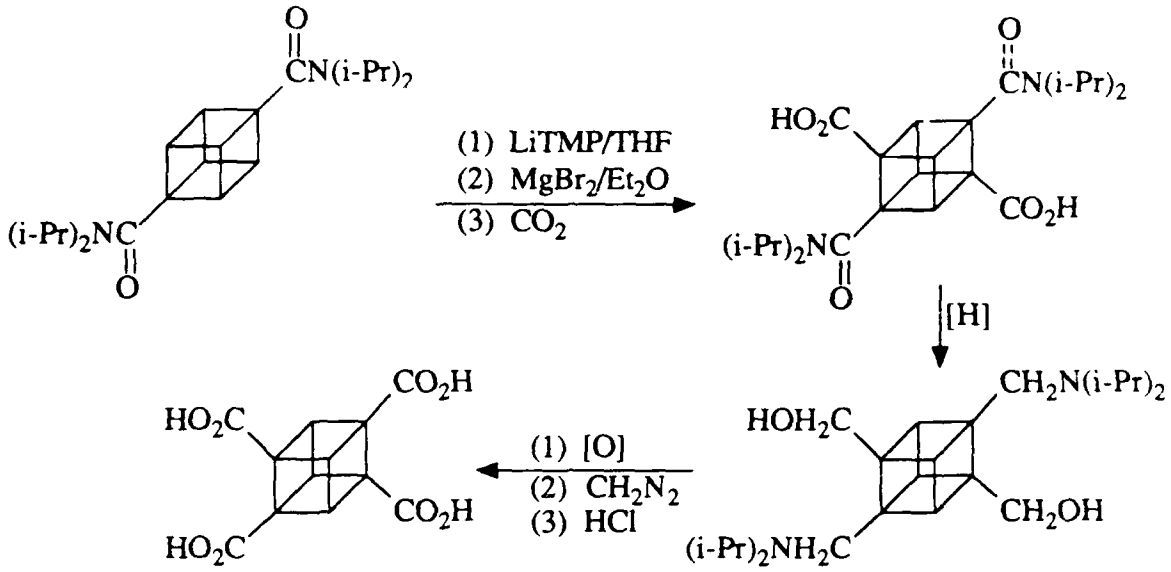
RESULTS

NEW SYNTHESIS OF CUBANE-1,2,4,7-TETRACARBOXYLIC ACID

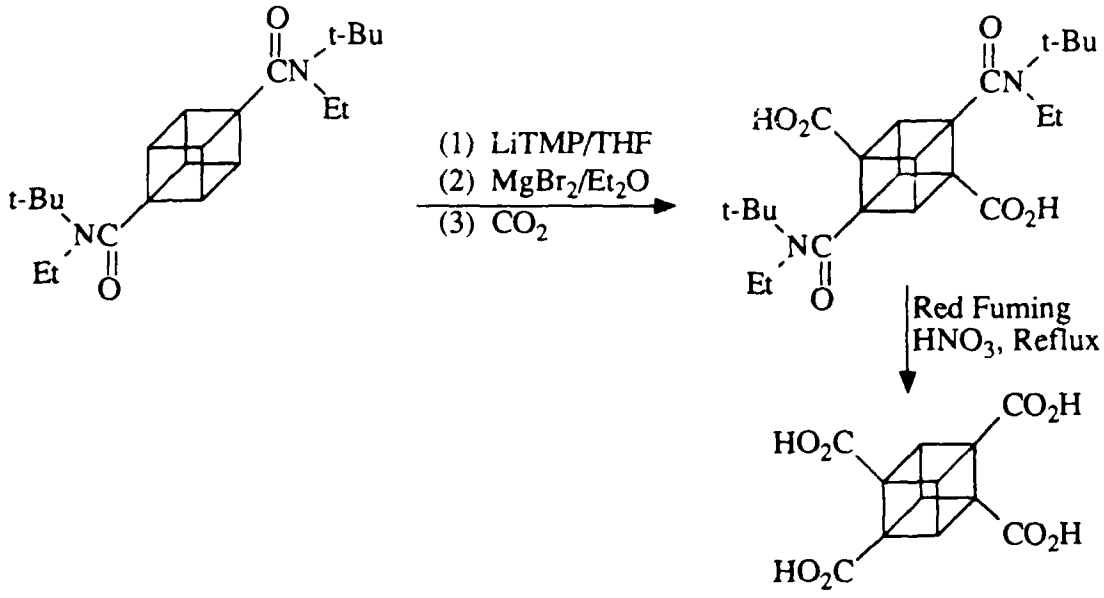
The large number of steps in the current synthesis of cubane-1,2,4,7-tetracarboxylic acid, a route initially developed by P. Eaton limits the ability to scale-up its synthesis. We have developed a new, simpler synthesis for this intermediate. Both syntheses are shown in Figure 1. The crucial factor in our synthetic route is the discovery that a different amide, ethyl, t-butylamide, can successfully be used in place of diisopropylamide in the ortho lithiation of the cubane nucleus. Not only does this new cubyl amide give a higher yield than the diisopropylamide for the lithiation step, but we can remove the ethyl, t-butylamide nearly quantitatively in one step and thus isolate the cubane-1,2,4,7-tetracarboxylic acid from the reaction mixture as a solid. This improvement eliminates the need for the oxidation, reduction, methylation, and demethylation sequence previously required to isolate the cubane-1,2,4,7-tetracarboxylic acid from the cubane-1,4-diisopropylamide-2,7-diacid.

We have not yet explored all the ramifications of this change in the overall procedure for the synthesis of cubane-1,2,4,7-tetracarboxylic acid, we do not yet know whether the use of this new cubyldiamide may allow the use of less expensive materials than tetramethylpiperidine the lithiation step as well as for other, equally complicated transformations.

Table 1, shows several different amides we explored as replacements for diisopropylamide before discovering the one that is serving us so well. We should point out that all the metallations listed in Table 1 (except that with ethyl, t-butylamide) were done before the metallation procedure using $MgBr_2$/etherate was invented by Bashier Hashimi of ARDEC and became available. We do not expect that any of these amides will work better with Hashimi's metallation procedure, so we do not now plan to reinvestigate these derivatives.



(a): Current synthesis developed by P. Eaton.



(b): Improved synthesis, developed by SRI International

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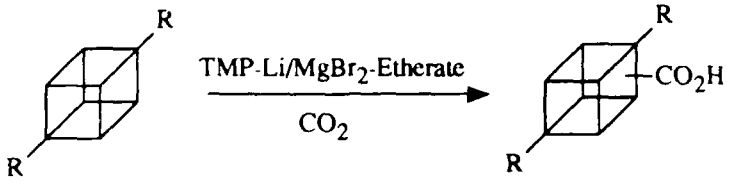
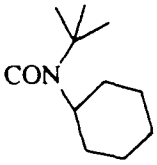
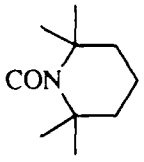
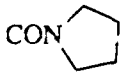
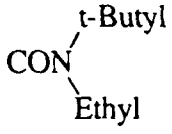
Figure 1. Current method and new, simpler method for synthesizing cubane-1,2,4,7-tetracarboxylic acid.

Table 1

ATTEMPTED METALLATIONS OF CUBANE

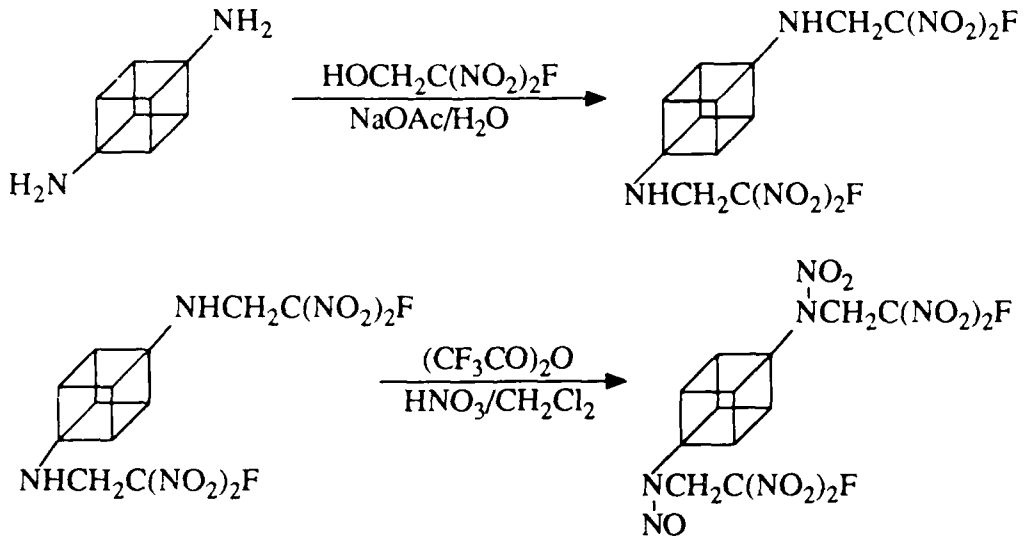


R	Carboxylation Observed (Yield)
	None
	None
	None
	None
	75%

NEW OXIDIZERS AND EXPLOSIVES

Polynitro Derivatives of Aminocubane

We have succeeded in synthesizing the first polynitro cubane compounds. The derivatives we prepared have nitro groups substituted at the amino group of a cubane. Clearly, these compounds are only intermediate targets along the pathway to the synthesis of cubanes that are nitrated on the cage. The first amino substituted cubane we prepared was bis-N,N'-(ß,ß-dinitro-ß-fluoroethyl)-1,4-diaminocubane which was then further nitrated to give the second, N-nitro-N'-nitroso-bis-N,N'-(ß,ß-dinitro-ß-fluoroethyl)-1,4-diaminocubane, as shown below.



The density of N-nitro-N'-nitroso-bis-N,N'-(β,β–dinitro-β-fluoroethyl)-1,4-diaminocubane is 1.827 g/cm^3. Its structure is shown in Figure 2.

Our simple KJSM calculations indicate that N-nitro-N'-nitroso-bis-N,N'-(β,β-dinitro-β-fluoroethyl)-1,4-diaminocubane has a detonation pressure (P_{CJ}) of 351 kbar and a detonation velocity (D_{vel}) of 8.9 mm/µsec. These values compare favorably to those of HMX, the best oxidizer currently used. HMX has a P_{CJ} of 371 kbar and a D_{vel} of 9.0 mm/µsec as calculated by the KJSM method. The calculated detonation properties of N-nitro-N-nitroso-bis-N,N'-(ß,ß-dinitro-ß-fluoroethyl)-1,4-diaminocubane are surprisingly good when one considers that the molecule does not contain enough oxygen to completely

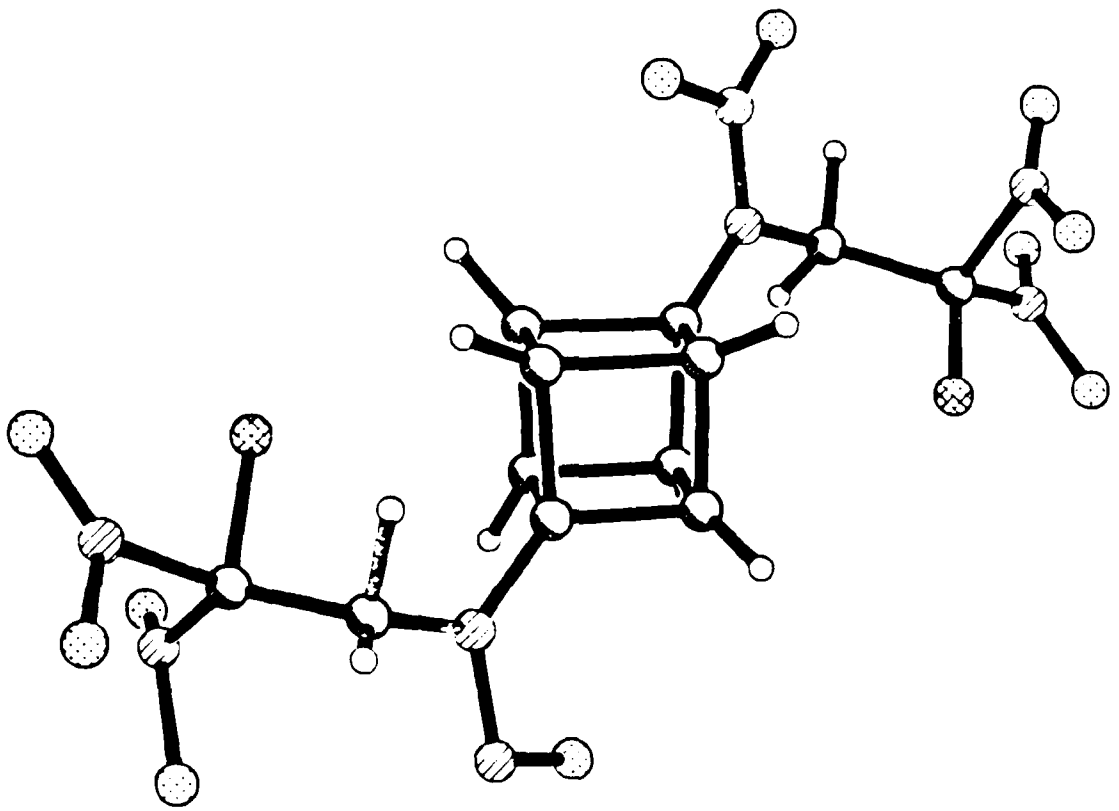


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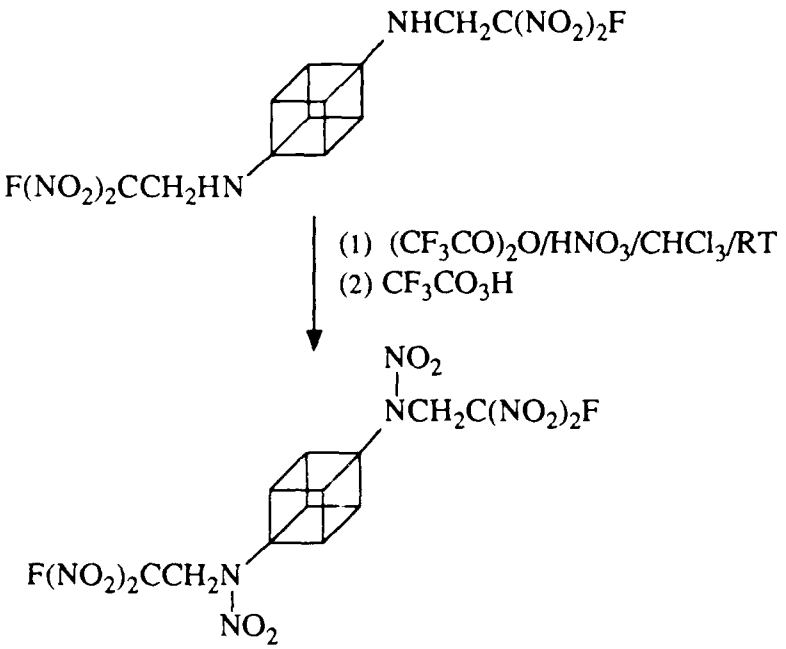
Figure 2. N-Nitro-N'-nitroso-bis-N,N'-(β,β-dinitro-β-fluoroethyl)-1,4-diaminocubane Density = 1,827 g/cm^3. Crystal structure by R. Gilardi and J. Flippen-Anderson of the Naval Research Laboratory.

oxidize all of the carbon and hydrogen to CO and water upon combustion. These excellent detonation properties are an example of the effect of adding a cubane nucleus into the molecule: both the density and the heat of formation are markedly increased, and these increases result in the high P_{CJ} and D_{vel}.

In our recent work, we have succeeded in synthesizing the fully oxidized derivative, N,N'-dinitro-bis-N,N'-(ß,ß-dinitro-ß-fluoroethyl)-1,4-diaminocubane by oxidation of the initially formed product as shown below.



The results of differential scanning calorimetry (DSC) for N,N'-dinitro-bis-N,N'-(β,β-dinitro-β-fluoroethyl)-1,4-diaminocubane are shown in Figure 3. This compound is a good example of what can be done with the cubane nucleus to enhance its energetic properties by simple chemistry.

A remarkable aspect of these compounds is that both N,N'-dinitro-bis-N,N'-(ß,ß-dinitro-ß-fluoroethyl)-1,4-diaminocubane and N-nitro-N'-nitroso-bis-N,N'-(ß,ß-dinitro-ß-fluoroethyl)-1,4-diaminocubane are more stable than bis-N,N'-(ß,ß-dinitro-ß-fluoroethyl)-1,4-diaminocubane. The aminocubane system is itself unstable and eventually decomposes via opening of the cubane ring system through donation of the free electron pair of the amino group into the cubyl cage. The N-nitro groups stabilize the aminocubane system by withdrawing electron density from the amino group; this withdrawal prevents the lone pair

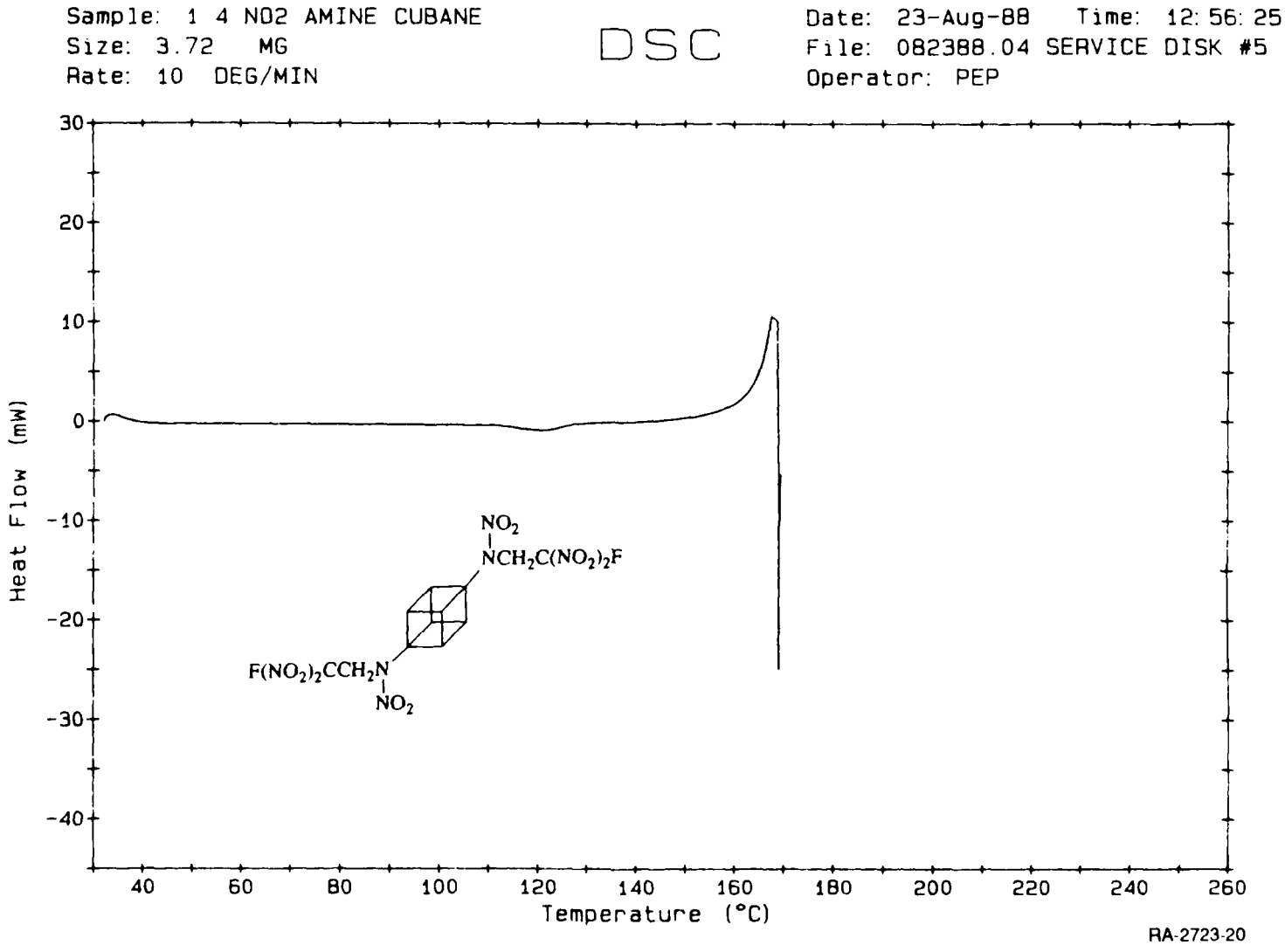
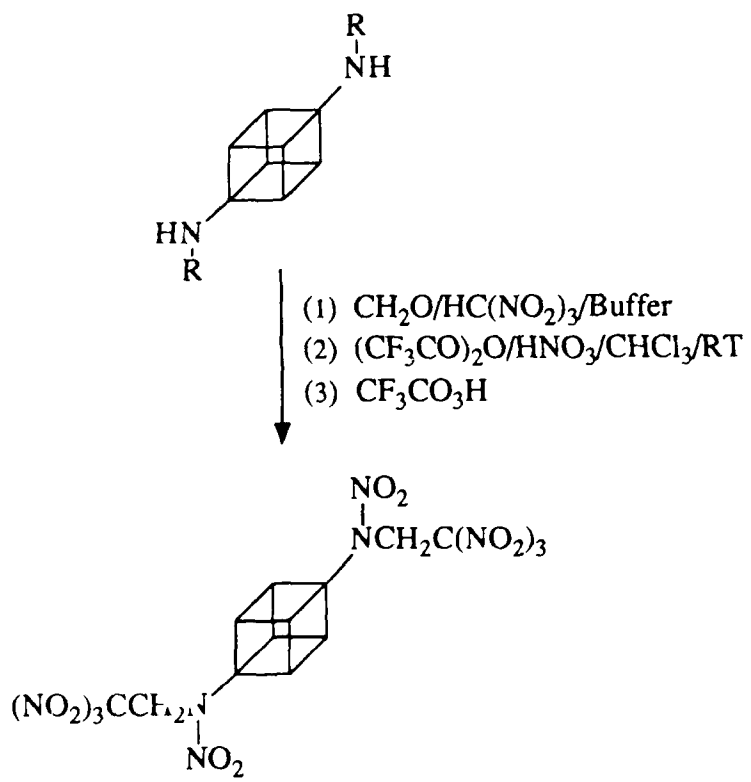


Figure 3. DSC for N,N'-dinitro-bis-N,N'-(β,β-dinitro-β-fluoroethyl)-1,4-diaminocubane.

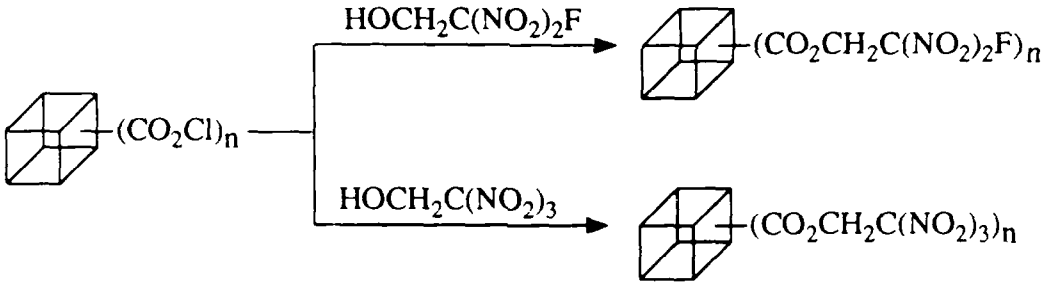
of electrons on the amino group from being donated into the cage and catalyzing its decomposition. This is an important observation because it indicates that N-nitro-amino-cubanes or aminocubanes with strongly electron withdrawing groups on the amino group will be stable.

We are working on the synthesis of the analogous bis-1,4-(ß,ß,ß-trinitro-ethyl-amino)cubane. This compound is of interest due to its considerably higher heat of formation and greater oxygen density. We have found in our initial attempts that the $NHCH_2C(NO_2)_3$ group on a cubane is not stable but loses formaldehyde to give a cubyl trinitromethide salt, cubyl-$[NH_3^+C(NO_2)_3^-]_2$, as the product. We are currently investigating alternative routes to this compound that involve first protecting the amino group with an electron withdrawing group such as an acetyl to stabilize the amine/formaldehyde addition product and then N-nitrating to give the desired product. This route is shown below.



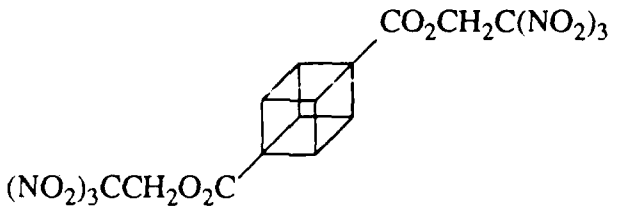
Cubane Esters of Trinitroethanol and Fluorodinitroethanol

We have also prepared cubane esters substituted with 2,2,2-trinitroethanol (TNE) and 2,2-dinitro-2 fluoroethanol (FDNE). These compounds give immediate access into very highly nitrated cubanes that are oxidized to $CO/H_2O/N_2$ and beyond. These compounds represent the first examples of fully oxidized cubanes.

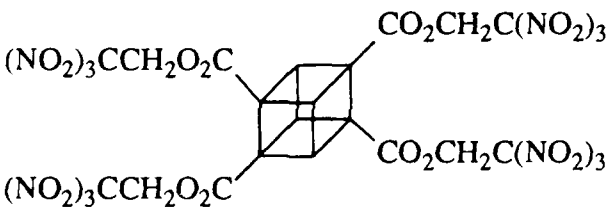


where n = 2 or 4.

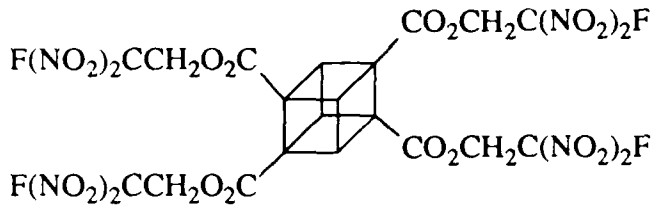
We have thus far synthesized three of the possible polynitro esters: cubane-1,4-bis(ß,ß,ß-trinitroethylester), cubane-1,2,4,7-tetrakis(ß,ß,ß-trinitroethylester) and cubane-1,2,4,7-tetrakis(ß,ß-dinitro-ß-fluoroethylester). Structures of these compounds are shown below.



Cubane-1,4-bis(ß,ß,ß-trinitroethylester)



Cubane-1,2,4,7-tetrakis(ß,ß,ß-trinitroethylester)

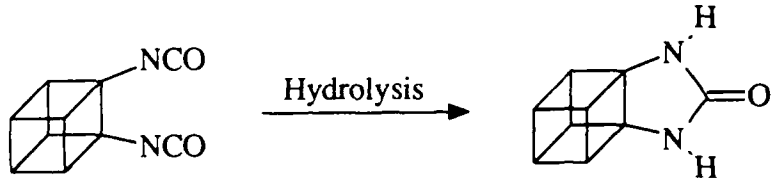


Cubane-1,2,4,7-tetrakis(ß,ß-dinitro-ß-fluoroethylester)
Density = 1.762 g/cm^3

Figure 4 shows the DSC for cubane-1,4-bis(β,β,β-trinitroethylester). Cubane-1,2,4,7-tetrakis(ß,ß-dinitro-ß-fluoroethylester) and cubane-1,2,4,7-tetrakis(ß,ß,ß-trinitro-ethylester) represent the first examples of potentially useful energetic materials made from a cubane nucleus. Cubane-1,2,4,7-tetrakis(ß,ß,ß-trinitroethylester) is over-oxidized and is an energetic powerhouse. The x-ray crystal structure (Figure 5), done by Dr. Richard Gilardi of the Naval Research Laboratory, of cubane-1,2,4,7-tetrakis(ß,ß-dinitro-ß-fluoroethylester) confirms our structure for the molecule and gives a crystal structure density of 1.762 g/cm^3. Figure 6 shows the DSC for this compound.

Propellanocubane Nitration.

A synthesis of the propellanocubane (below) has recently been worked out in Professor Eaton's laboratory.



We have been studying the nitration of this interesting intermediate with the goal of synthesizing the tetra-N-nitro derivative of the bis-propellanocubane, a cubane equivalent of TNGU. Initially, we synthesized the bis-TMS derivative by reacting TMS-Cl/base with propellanocubane. The goal here was to prepare a protected version of the propellanocubane with improved solubility. All attempts at nitration of this intermediate and direct nitration of propellanocubane have failed thus far to result in the bis-N-nitro-propellanocubane we seek. Further studies will be done to attempt to solve this problem

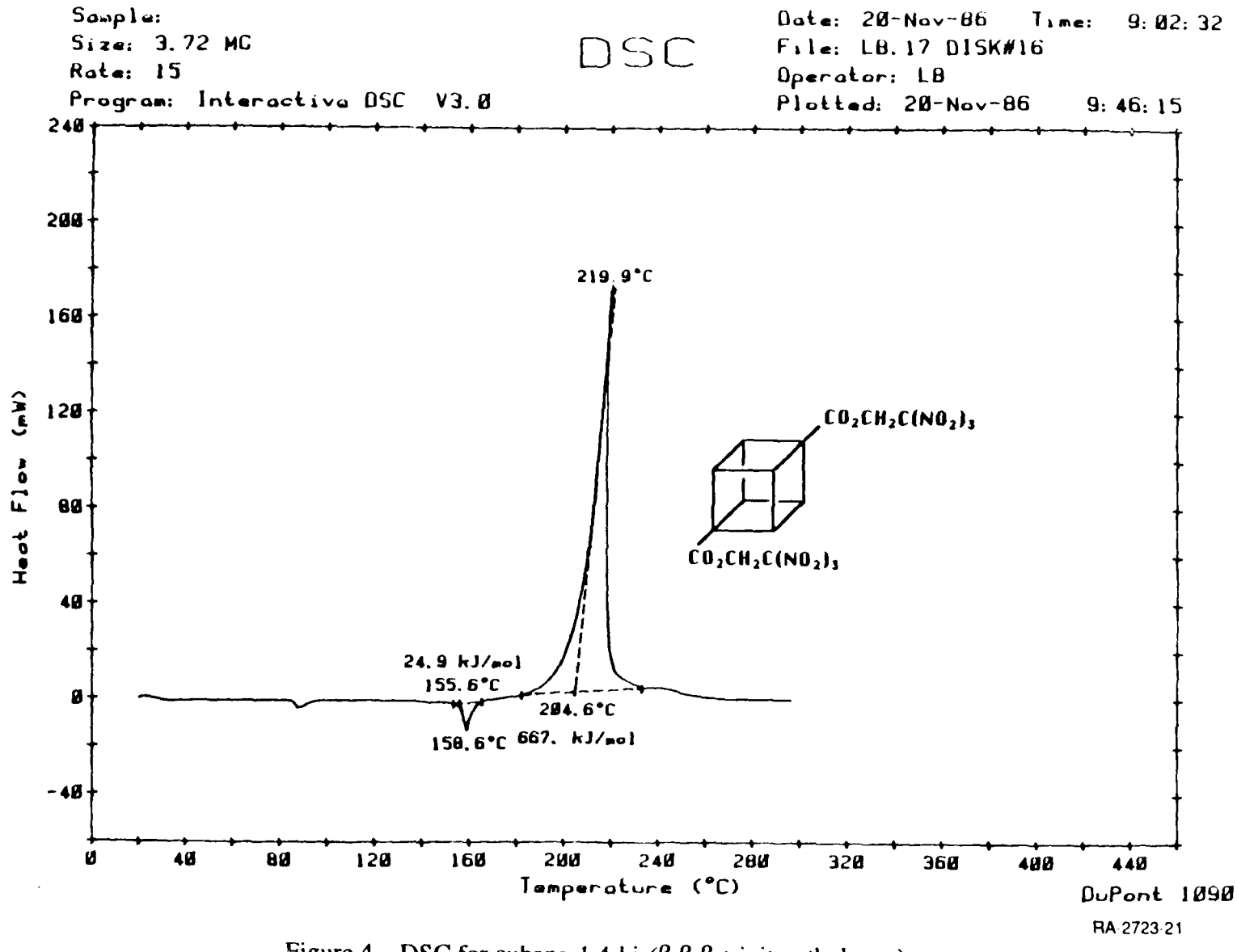


Figure 4. DSC for cubane-1,4-bis(β,β,β-trinitroethylester).

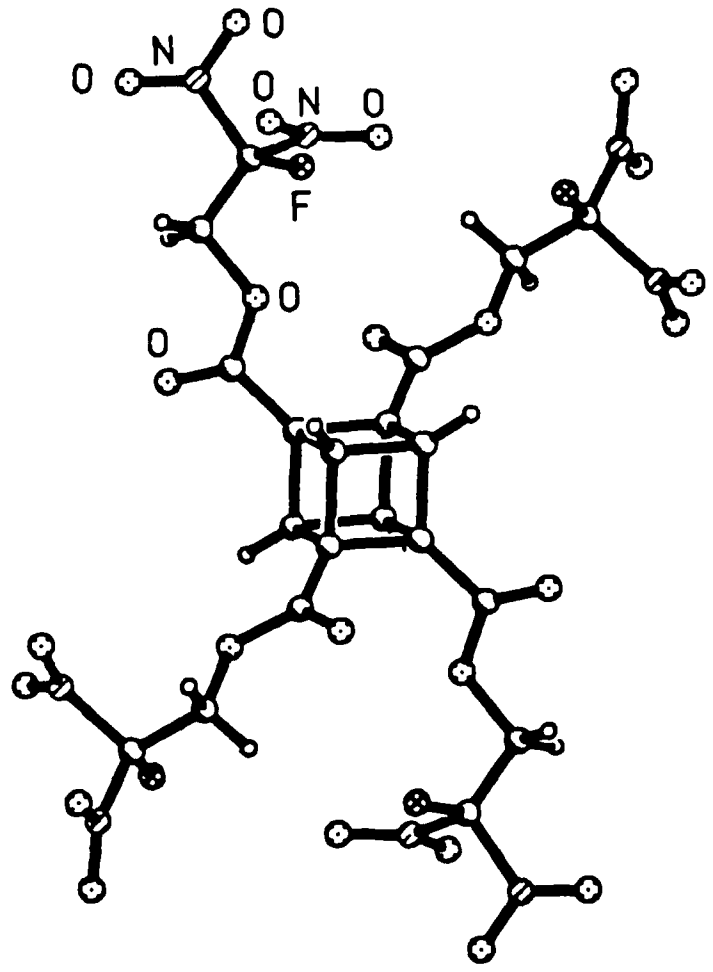


Figure 5. Cubane-1,2,4,7-tetrakis(β,β-dinitro-β-fluoroethylester). Density = 1,762 g/cm^3. Crystal structure by R. Gilardi and J. Flippen-Anderson of the Naval Research Laboratory.

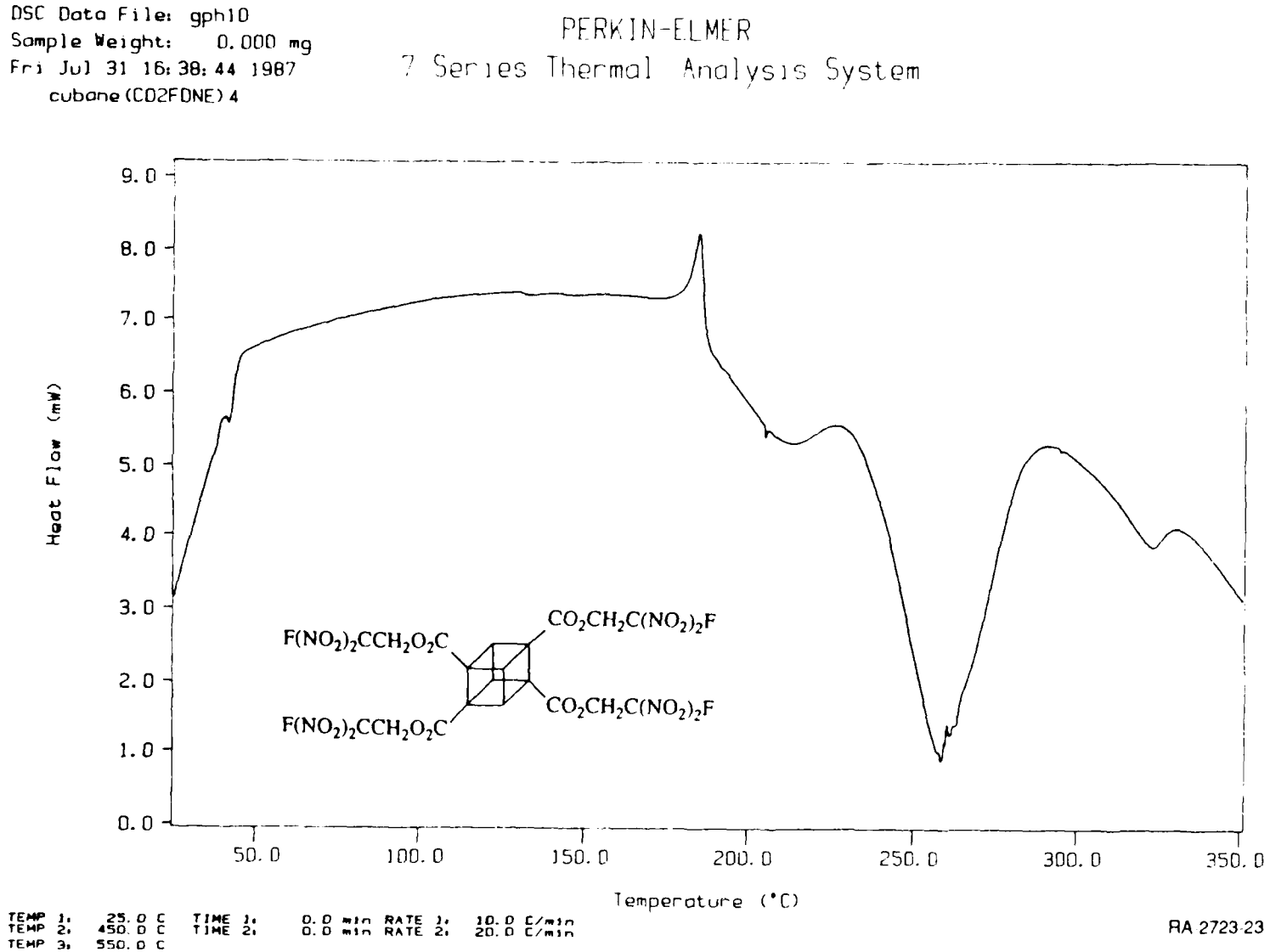
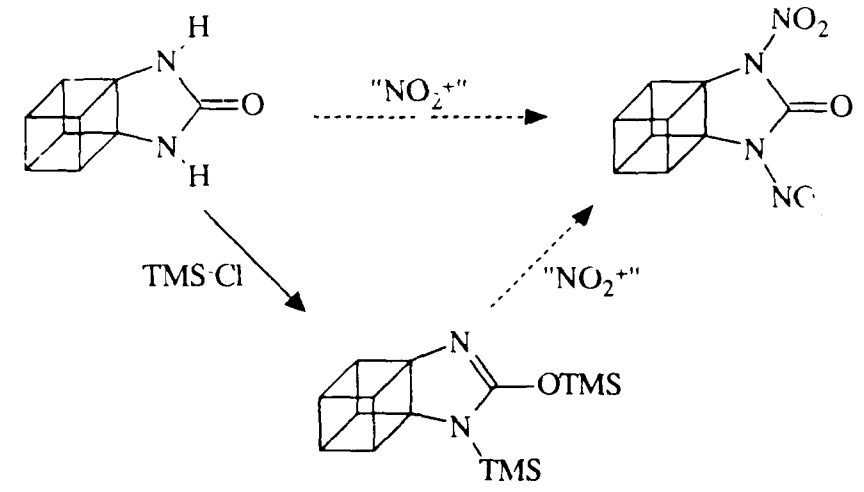
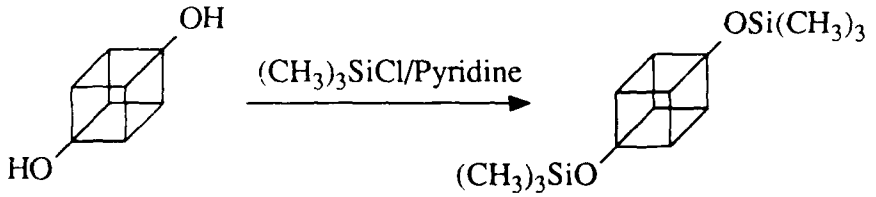


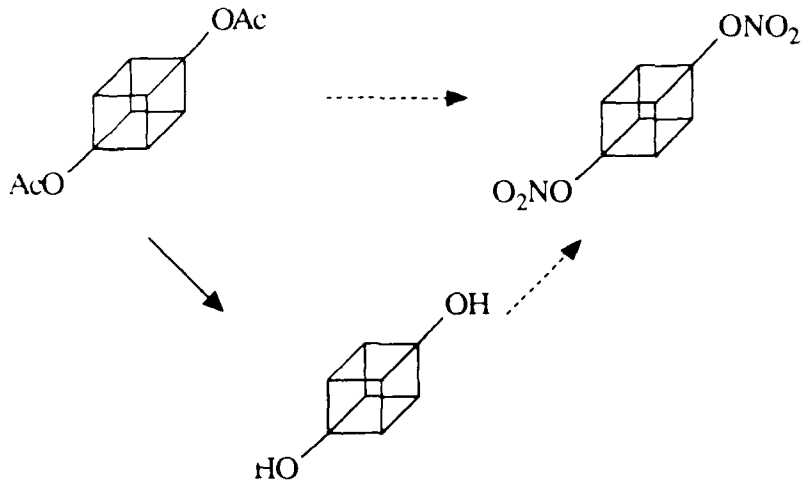
Figure 6. DSC for cubane-1,2,4,7-tetrakis(β,β-dinitro-β-fluoroethylester).



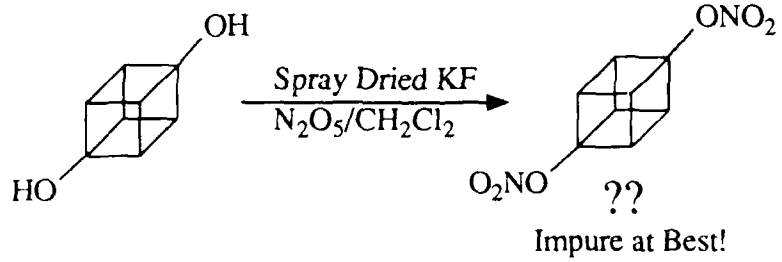
Synthesis of Cubylnitrates

The recent synthesis of cubane-1,4-diol by Eaton has led us to attempt the synthesis of cubane-1,4-dinitrate from the diol. We were initially encouraged by our success in synthesizing 1,4-bis(trimethylsiloxy)cubane from the diol (as shown below) under conditions similar to those required for the synthesis of the nitrate.





However, we have not yet been able to synthesize the cubane-1,4-dinitrate as expected. Our initial results from the reaction of the 1,4-cubanediol with KF/N_2O_5 in CH_2Cl_2 indicate that we have indeed synthesized the dinitrate. This is demonstrated by a shift of the cubyl protons from 3.8 ∂ (s) for the diol to 4.3 ∂ (s) for the suspected dinitrate. The IR spectrum shows the presence of both of the expected peaks for nitrate at 1680 and 1450 cm^{-1}, exactly as expected for the dinitrate. However, these samples were impure, and we have not yet been able develop a purification procedure in which the presumed dinitrate survives. Because this is quite a desirable compound, we are continuing attempts toward its synthesis.

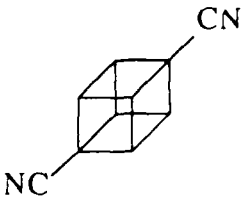


Impure at Best!

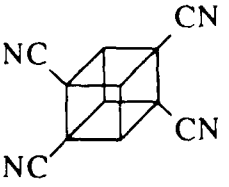
NEW FUELS

Polycyanocubanes

We have started work on the synthesis of polycyanocubanes for use as dense, high energy rocket fuels. For example, octacyanocubane is calculated to have a heat of formation (ΔH_f) of +395 kcal/mol and a density greater than 1.5 g/cm^3. Each cyano group contributes 30.9 kcal/mol to the ΔH_f formation of the molecule. Thus, the cyanocubanes would be ideal energy dense fuels for volume limited applications. We have synthesized 1,4-dicyanocubane the (DSC for which is shown in Figure 7, and are synthesizing 1,2,4,7-tetracyanocubane as another example of these compounds. The structures and ΔH_f of these two compounds are shown below. We will prepare the rest of the cyanocubanes as we proceed in this program.



1,4-Dicyanocubane
ΔH_f (calc) = 191 kcal/mol



1,2,4,7-Tetracyanocubane
ΔH_f (calc) = 253 kcal/mole

Cubane-1,4-diisocyanide

The isocyanides are especially interesting as energy increasing groups. Isocyanocubanes, like the polycyanocubanes, should make extremely good fuels or fuel additives for propellant applications because of their high positive ΔH. The isocyanide group is even more energy dense than the cyano group and thus even more energy is obtained for the same weight of compound. Each isocyanide group contributes +45.8 kcal/mol to the ΔH_f a very dramatic increment.

We recently synthesized cubane-1,4-diisocyanide by reacting cubane-1,4-diisocyanate with Cl_3SiH in Et_3N as shown below.

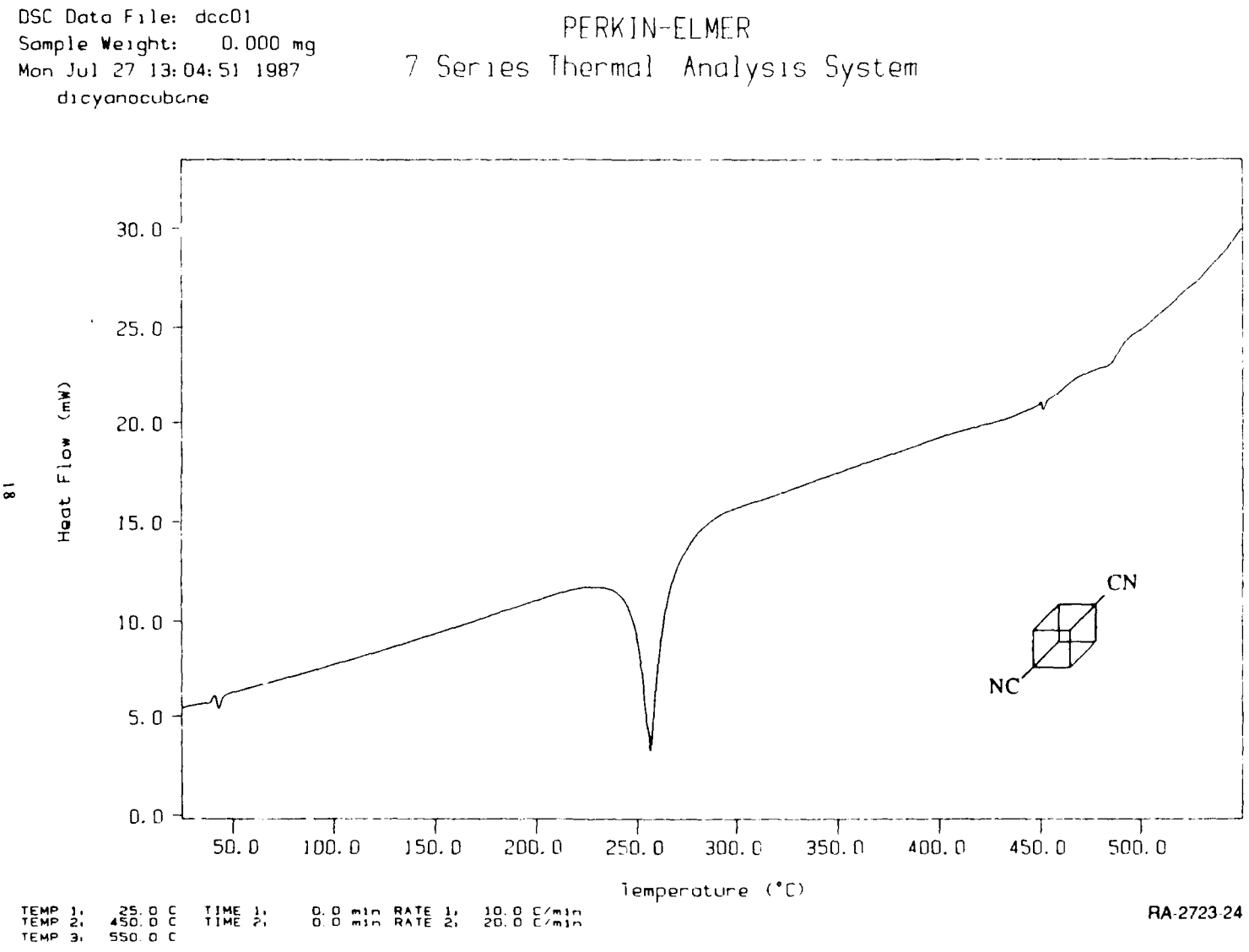
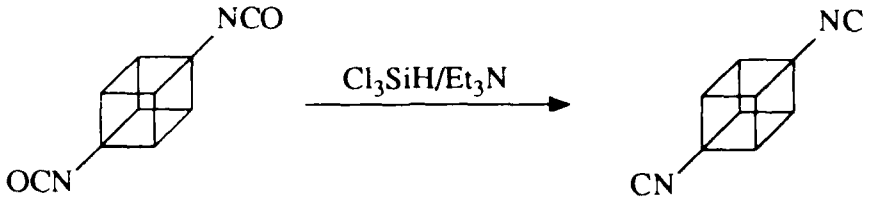


Figure 7. DSC for 1,4-dicyanocubane.



cubane-1,4-diisocyanate
ΔH_f (calc) = +221 kcal/mol

Cubane-1,4-diisocyanide is calculated to have a ΔH_f of +221 kcal/mol, an extremely high value for a compound containing only C, H, and N.

CALCULATIONS OF CUBANE DERIVATIVES HEAT OF FORMATION, DENSITY, AND SPECIFIC IMPULSE

We have calculated the ΔH_f, density, and specific impulse (I_{sp}) of various cubane derivatives to evaluate their potential performance as rocket propellants and explosives. Table 2 summarizes the results of these calculations. The accuracy, of these calculations were checked by independent calculations performed by Dr. Rodney Willer of the Elkton Division of Morton Thiokol.

Several assumptions were made in the calculations. The ΔH_f was calculated using Benson group additivity with cubane as the base. The ΔH_f of cubane in the solid state, taken to be 129 kcal/mol, was used as the starting point for these calculations and the group heats of formation were added to it. Energetic groups were calculated using the ΔH_f for such groups provided by the Naval Weapons Center, China Lake. No vicinal interactions were included the calculations, because these interactions will be minimized because of the geometry of cubanes. The calculations of ΔH_f are shown in appendix A.

The densities were calculated by the Holden method and the Stine method and are listed in Appendix B. In the Holden calculations we assumed 3 rings instead of 5 rings, because this assumption gives the correct densities for cubane, dinitrocubane, and dinitraminocubane.

Specific impulse (I_{sp}) was calculated using the NASA-Lewis code unmodified and the calculated heats of formations.

Table 2
Estimated Parameters for Various Tetrasubstituted Cubanes[a]

Energetic Group	Molecular Formula	Density (g/cm^3)	ΔH_f (kcal/mol)	P_{CJ} (kbar)	D_{vel} (μm/sec)	Monopropellant I_{sp} (sec)	Monopropellant $I_{sp}*\rho^{3/4}$ (sec)
NO_2	$C_8H_4N_4O_8$	1.87	+71	308	8.25	250	400
ONO_2	$C_8H_4N_4O_{12}$	1.94	+33	376	9.01	274	450
$NHNO_2$	$C_8H_8N_8O_8$	1.86	+160	335	8.61	261	416
$N(NO_2)_2$	$C_8H_4N_{12}O_{16}$	2.02	+250	470	9.91	283	480
$C(NO_2)_3$	$C_{12}H_4N_{12}O_{24}$	1.96	+40	403	9.30	264	437
NF_2	$C_8H_4N_4F_4$	1.92	+103	-	-	246	401
$N(NO_2)CON(NO_2)$	$C_8H_4N_8O_{10}$	2.01	+108	352	8.63	243	410
$OClO_3$	$C_8H_4Cl_4O_{16}$	>2	+100	-	-	262	440
$N(NO_2)CH_2N(NO_2)_2$	$C_{16}H_{12}N_{20}O_{32}$	1.89	+70	378	9.1	270	435
$N(NO_2)CH_2C(NO_2)_2F$	$C_{16}H_{12}N_{16}O_{24}F_4$	1.86	-77	360	8.92	265	422
$CO_2CH_2C(NO_2)_3$	$C_{20}H_{12}N_{12}O_{32}$	1.90	-308	337.5	8.6	242	392
$CO_2CH_2C(NO_2)_2F$	$C_{20}H_{12}N_8O_{24}F_4$	1.90	-455	286.5	7.9	214	346
HMX	$C_4H_8N_8O_8$	1.90	+17.9	390	9.1	265	429
XX	$C_6H_6N_{12}O_{12}$	1.98	+101	430	9.58	272	454
Ammonium Perchlorate	NH_4ClO_4	1.95	-71	-	-		
HAP	NH_4ClO_5	2.07	-66	-	-		

[a]Densities calculated using the method of Holden, ΔH_f calculated using Benson group additivity, P_{cj} and D_{vel} calculated using the KJSM method, and I_{sp} calculated using the NASA-Lewis code.

X-RAY CRYSTAL DATA

X-ray crystal structures were done on several of the compounds prepared for this program. All structural determinations were performed by Dr. Richard Gilardi of the Naval Research Laboratory. We have included the results of one of these x-ray studies as Appendix C.

EXPERIMENTAL PROCEDURES

Cubane-1,4-bis(ethyl, t-butylamide). Cubane-1,4-dicarboxylic acids were reacted with excess purified thionyl chloride and, the residual thionyl chloride distilled off. This procedure left cubane-1,4-diacid chloride as the product. Cubane-1,4-diacid chloride was reacted with 2 g of ethyl, t-butylamine. A vigorous reaction ensued, and the reaction mixture was stirred for 3 hours at room temperature. The reaction mixture was diluted to 40 mL with $CHCl_3$ and extracted once with 20 mL of 10 M NaOH. The organic layer was concentrated in vacuo. The product was crystallized from ethyl acetate to give 600 mg of clear colorless plates. NMR (^1H, $CDCl_3$, TMS standard) ∂ 1.3 (triplet, 3 H, J = 7 Hz), ∂ 1.4 (S, 9H, t-butyl), ∂ 3.8 (quartet, 2H, J = 7 Hz, CH_2), ∂ 4.55 (S, 6H); IR (KBr) 2970, 1610, 1390, 1205 cm^{-1}; mp = 187°C.

Cubane-1,2,4,7-tetracarboxylic acid. Cubane-1,4-bis(ethyl, t-butylamide) was carboxylated exactly like the corresponding diisopropylamide in the method developed by Eaton Associates and Bashir Hashemi of ARDEC. Cubane-1,4-bis(ethyl, t-butylamide) (360 mg, 1.0 mmol) was added to a preformed mixture of TMEDA (1.2 g, 10 mmol), THF (10 mL), $MgBr_2$ (1.25 g, 0.5 mmol), and lithium tetramethylpiperidide (from 1.40 g, 10 mmol of tetramethylpiperidine and 10 mmol of n-butyl-lithium) at 0°C. After the mixture was stirred for 3 hours at 0°C, all the solid had sdissolved. The reaction mixture was stored for 36 hours at 0°C and then placed under an atmosphere of dry CO_2 and stirred at room temperature for 2 hours. All volatiles were removed in vacuo. The residue was suspended in 100 mL of H_2O and acidified with dilute (2 M) HCl to a pH of 3. White crystals precipitated and were collected by filtration to give the intermediate diacid, diamide (300 mg, 0.6 mmol, 60%). This material (100 mg, 0.25 mmol) was refluxed in 5 mL of 90% HNO_3 for 5 hours and then, evaporated to dryness in vacuo, to give 43 mg (65%) of white crystals of cubane-1,2,4,7-tetracarboxylic acid. ^1H NMR (CD_3OD) ∂ 4.3 (s).

Cubane-1,2,4,7-tetrakis(ß,ß,ß-trinitroethylester).

Cubane-1,2,4,7-tetracarboxylic acid (15 mg, 0.05 mmol) was stirred with 0.5 g PCl_5 in 4 mL of 1,2-dichloroethane for 24 hours under argon. The resulting solution was treated with 250 mg of Ac_2O,and then freed of volatile materials by careful distillation under high vacuum. At the end of the distillation, the residue was heated to 75°C for 5 minutes. The crude tetraacid chloride, which was a yellow oil, was combined with 100 mg (0.6 mmol) of rigorously dried 2.2,2-trinitroethanol and 2 mL of 1:1 EtOAc/$CHCl_3$. Pyridine (50 mg, 0.6 mmol) was added, and the entire mixture was sealed under argon and stirred for 3 days. The reaction mixture was dissolved in 50 mL of EtOAc and extracted with 50 mL of 10% Na_2CO_3, concentrated, and chromatographed over 20 g of SiO_2, being eluted with 1:1 EtOAc/CHCl3. The $R_f = 0.7$ material was collected and found to be crystalline, with a mass of 4.0 mg. This material was crystallized from EtOAc/$CHCl_3$ to give 2 mg of crystals (~5% yield). ^1H NMR (D_6-acetone, TMS standard, 400 MHz) ∂ 5.9 (s, 8 H, CH_2), ∂ 4.6 (s, 4H, C-H); ^{13}C NMR (D_6-acetone) ∂ 48.7, ∂ 56.2, ∂ 61.8, ∂ 165.2. IR (KBr) 2995, 1730, 1600, 1300, 1200, 1185, 1065 cm^{-1}.

Cubane-1,2,4,7-tetrakis(ß,ß-dinitro-ß-fluoroethyl ester). The procedure used for the the synthesis of the ß,ß,ß-trinitroethylester was followed on double the scale, fluorodinitro-ethanol substituted for the trinitroethanol. Cubane-1,2,4,7-tetrakis(ß,ß-dinitro-ß-fluoroethylester), 1 mg (8%), isolated as needles. ^1H NMR (D_6-acetone, TMS standard, 60 MHz) ∂ 4.7 (s, 4 H, C-H), ∂ 5.65 (d, j = 15 Hz, 2 H, CH_2). The x-ray crystal structure determined by R. Gilardi of NRL gave a density of 1.827 g/cm^3. The x-ray crystal structure and structural parameters are included in Appendix C.

Bis-N,N'-(ß,ß-dinitro-ß-fluoroethyl)diaminocubane. 1,4-Diamino-cubane hydrochloride (200 mg, 0.95 mmol), prepared by the method of Eaton, was dissolved in 10 mL of H_2O and treated with purified 2-fluoro-2,2-dinitroethanol (900 mg, 6 mmol) followed by sodium acetate (700 mg, 8 mmol) for 12 hours at room temperature. An orange precipitate was isolated by filtration, dissolved in EtOAc and filtered through a 2-inch by 1/2-inch plug of silica gel, concentrated, and crystallized from $CHCl_3$/EtOAc to give 180 mg (45%) of needles of N,N'-bis-N,N'-(ß,ß-dinitro-ß-fluoroethyl)diamino-cubane. ^1H NMR(D_6-acetone TMS standard, 60 MHz) ∂ 3.7(s, 6 H, C-H), ∂ 4.0-4.5 (m, 6 H, CH_2 + NH); IR (KBr) 3375, 3000, 1630, 1600, 1585, 1330 cm^{-1}.

N-Nitro-N'-nitroso-bis-N,N'-(ß,ß-dinitro-ß-fluoroethyl)-1,4-diaminocubane. Bis-N,N'-(ß,ß-dinitro-ß-fluoroethyl)-1,4-diaminocubane (60 mg, 0.15

mmol) was dissolved in 5 mL of $CHCl_3$ and added to a preformed solution prepared by combining trifluoroacetic anhydride (400 mg, 2 mmol) with 100% HNO_3 (180 mg, 3 mmol) at 0°C, stirring for 10 minutes, and then diluting with 5 mL $CHCl_3$. The resulting mixture was stirred at 0°C for 15 minutes, warmed to 20°C, diluted with 50 mL of $CHCl_3$, and concentrated in vacuo. The residue was chromatographed, using ethyl acetate over SiO_2 for elution, and the fastest effluen was collected. The resulting material was crystallized from ethyl acetate/$CHCl_3$ to give 30 mg of crystals. mp = XX°C; ^1H NMR (D_6-acetone, TMS standard, 90 MHz) ∂ 4.1-4.8 (m, 6 H), ∂ 5.2-6.2 (m, 4 H, CH_2); IR (KBr) 3040, 1630, 1560, 1460, 1415, 1310, 1290, 1170 cm^{-1}. The x-ray crystal structure determined by R. Gilardi of NRL gave a density of 1.827 g/cm^3.

N,N'-Dinitro-bis-1,4-(ß,ß-dinitro-ß-fluoro-ethyl-amino)-cubane. The N-nitro-N'-nitroso-bis-1,4-(ß,ß-dinitro-ß-fluoroethylamino)cubane described above (50 mg, 0.11 mmol) was dissolved in a 0.5 M solution of CF_3CO_3H in 1:1 $CHCl_3$/EtOAc and stirred for 36 hours. The reaction mixture was diluted to 100 ml with HPLC grade ethyl acetate, extracted with 50 mL of 1 M Na_2SO_3, dried, and concentrated in vacuo to give 50 mg (95%) of pure dinitramine as white plates. ^1H NMR (D_6-acetone, TMS standard 90 MHz) ∂ 4.4 (s, 6 H, C-H), ∂ 5.65 (d, J = 14 Hz, 4 H, CH_2), IR (KBr) 3000, 1625, 1555, 170°C 1280 cm^{-1}, mp = 170°C (explodes).

Cubane-1,4-diol. Cubane-1,4-diacetate (100 mg, 0.4 mmol) was dissolved in 25 mL of HPLC grade $CHCl_3$ and cooled to 0°C under an argon blanket. Diisobutyl aluminum hydride (2 mmol of a 1.5 M solution in toluene) was added and the resulting mixture was stirred for 30 minutes. Ethyl acetate (50 mL) was added, and 4 mL of 2 M NaH_2PO_4 was then added to destroy all organoaluminum species. The mixture was stirred until all organoaluminum species had precipitated out (~2 hr). The organic layer was decanted, the inorganic paste that remained was washed and stirred with 50 mL of EtOAc, and both organic layers were concentrated in vacuo to give a white powder that was titurated with $CHCl_3$ to give 50 mg (80%) of cubane-1,4-diol. mp = 150°C (decomposition); IR (KBr) 3200, 2960, 1330, 1140, 1000, 930 cm^{-1}; ^1H NMR (CD_3OD, 60 MHz) ∂ 3.2 (s, C-H).

1,4-Bis(trimethylsiloxy)cubane. Cubane-1,4-diol (15 mg, 0.1 mmol) was suspended in 2 mL of hexamethyldisilazane. Chlorotrimethylsilane (0.2 mL) was added, and the resulting mixture was stirred for 24 hours. Diethylamine (0.5 mL) was added to quench excess chlorotrimethylsilane. The mixture was evaporated to dryness in vacuo, redissolved in EtOAc, filtered to remove $Et_2NH_2^+Cl^-$, and concentrated to give 25 mg

(100%) of 1,4-bis(trimethylsiloxy)cubane, a waxy solid. ^{1}H NMR ($CDCl_3$) ∂ 3.85 (s, 6 H, C-H), ∂ 0.25 (s, 16 H, CH_3-Si).

1,4-Dicyanocubane. Cubane-1,4-diacid chloride (2.3 g, 10 mmol) was dissolved in 100 mL of $CHCl_3$ and treated with excess NH_3 gas until the exotherm subsided. The NH_3-saturated $CHCl_3$ was stirred for 2 hours at room temperature and concentrated in vacuo. A white solid product remained. The white solid was suspended in 100 mL of CH_2Cl_2 and treated with 10 mL of Et_3N plus 10 mL of $POCl_3$. This mixture was stirred for 3 days, concentrated in vacuo, freed of $POCl_3$ by chasing with chlorobenzene on a rotary evaporator, and partitioned between 200 mL of $CHCl_3$ and 100 mL of 10% Na_2CO_3. The $CHCl_3$ layer was kept. The crude product was chromatographed using 80% $CHCl_3$/20% EtOAc over silica gel for elution. The R_f = 0.5 material was collected as white prisms in a yield of 400 mg (25%). IR (KBr) 3060, 2260, 1290, 1230, 1220 cm^{-1}; ^{1}H NMR ($CDCl_3$, TMS standard, 60 MHz) ∂ 4.5 (s, C-H), mp = 225°C (explodes).

Cubane-1,4-diisocyanide. Trichlorosilane (1.7 g, 13 mmol) was dissolved in 15 mL of CH_2Cl_2, cooled to 0°C under argon, and treated with 3.7 g (30 mmol) of diisopropyl-ethylamine, followed by 1 g (5.5 mmol) of cubane-1,4-diisocyanate. The reaction mixture was stirred for 2 hours at 0°C, treated with excess ammonia gas to destroy the acidic chlorosilanes, partitioned between 400 mL of $CHCl_3$ and 400 mL of 1 M NaOH. The chloroform layer was dried, concentrated and flash-chromatographed eluting 1:1 EtOAc/$CHCl_3$ over a 3-inch by 1/2-inch plug of silica gel. The fastest effluent (R_f = 0.5) was collected and crystallized from hexane to give 20 mg (2%) of cubane-1,4-diisocyanide crystals. Decomposition > 125°C, detonating on rapid heating. IR (KBr) 3000, 2100, 1330 cm^{-1}; ^{1}H NMR ($CDCl_3$, TMS standard, 60 MHz) ∂ 4.3 (s).

CONCLUSIONS

We have developed a new, simpler method for functionalizing the cubane nucleus and have synthesized several polysubstituted cubanes as well as several members of a new class of energetic, high density fuels. We have found that the N-nitraminocubanes are more stable than the aminocubane system itself. We have also determined that the polycyanocubanes should make extremely good fuels or fuel additives because of their high positive heats of formation, and the isocyanocubares, with even higher heats of formation, should be even better for this use.

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Appendix A

CALCULATED HEATS OF FORMATION OF CUBANE DERIVATIVES

Appendix 1: Calculated Heat of Formation of Cubane Derivatives

Compound	Group Contribribution Contribribution	Number Of Groups	Subtotal	Calculated ΔHf
Cubanediacid				
Cubane	129.0	1	129.0	
$C(C_3)(H)$	-1.9	-2	3.8	
CO(C)(O)	-35.1	2	-70.2	
O(CO)(H)	-58.1	2	-116.2	
				-53.6
Cubane$(NO_2)_2$				
Cubane	129.0	1	129.0	
C(C3)(H)	-1.9	-2	3.8	
C(C3)(NO_2)	-16.5	2	-33.0	
				99.8
Cubane$(NO_2)_3$				
Cubane	129.0	1	129.0	
$C(C_3)(H)$	-1.9	-3	5.7	
$C(C_3)(NO_2)$	-16.5	3	-49.5	
				85.2
Cubane$(NO_2)_4$				
Cubane	129.0	1	129.0	
$C(C_3)(H)$	-1.9	-4	7.6	
$C(C_3)(NO_2)$	-16.5	4	-66.0	
				70.6
Cubane$(NO_2)_5$				
Cubane	129.0	1	129.0	
$C(C_3)(H)$	-1.9	-5	9.5	
$C(C_3)(NO_2)$	-16.5	5	-82.5	
				56.0
Cubane$(NO_2)_6$				
Cubane	129.0	1	129.0	
$C(C_3)(H)$	-1.9	-6	11.4	
$C(C_3)(NO_2)$	-16.5	6	-99.0	
				41.4
Cubane$(NO_2)_7$				
Cubane	129.0	1	129.0	
$C(C_3)(H)$	-1.9	-7	13.3	
$C(C_3)(NO_2)$	-16.5	7	-115.5	
				26.8

Cubane(NO_2)$_8$				
Cubane	129.0	1	129.0	
C(C_3)(H)	-1.9	-8	15.2	
C(C_3)(NO_2)	-16.5	8	-132.0	
				12.2
Cubane(ONO_2)$_2$				
Cubane	129.0	1	129.0	
C(C_3)(H)	-1.9	-2	3.8	
C-(C_3)(O)	-6.6	2	-13.2	
O-(C)(NO_2)	-19.4	2	-38.8	
				80.8
Cubane(ONO_2)$_3$				
Cubane	129.0	1	129.0	
C(C_3)(H)	-1.9	-3	5.7	
C-(C_3)(O)	-6.6	3	-19.8	
O-(C)(NO_2)	-19.4	3	-58.2	
				56.7
Cubane(ONO_2)$_4$				
Cubane	129.0	1	129.0	
C(C_3)(H)	-1.9	-4	7.6	
C-(C_3)(O)	-6.6	4	-26.4	
O-(C)(NO_2)	-19.4	4	-77.6	
				32.6
Cubane(ONO_2)$_5$				
Cubane	129.0	1	129.0	
C(C_3)(H)	-1.9	-5	9.5	
C-(C_3)(O)	-6.6	5	-33.0	
O-(C)(NO_2)	-19.4	5	-97.0	
				8.5
Cubane(ONO_2)$_6$				
Cubane	129.0	1	129.0	
C(C_3)(H)	-1.9	-6	11.4	
C-(C_3)(O)	-6.6	6	-39.6	
O-(C)(NO_2)	-19.4	6	-116.4	
				-15.6
Tetrakis(N-nitramino)cubane				
Cubane	129.0	1	129.0	
C-(C_3)(H)	-1.9	-4	7.6	
C-(C_3)(N)	-3.2	4	-12.8	
N-(NO_2)(H)(C)	9.5	4	38.0	
				161.8

Bis-(N(NO_2)FDNE)-Cubane				
Cubane	129.0	1	129.0	
C-(C_3)(H)	-1.9	-2	3.8	
C-(C_3)(N)	-3.2	2	-6.4	
N-(NO_2)(C_2)	17.8	2	35.6	
C-(N)(C)(H_2)	-6.6	2	-13.2	
C-(F)((NO_2)$_2$)(C)	-61.5	2	-123.0	
				25.8
Tetrakis-(N(NO_2)FDNE)-Cubane				
Cubane	129.0	1	129.0	
C-(C_3)(H)	-1.9	-4	7.6	
C-(C_3)(N)	-3.2	4	-12.8	
N-(NO2)(C_2)	17.8	4	71.2	
C-(N)(C)(H_2)	-6.6	4	-26.4	
C-(F)((NO_2)$_2$)(C)	-61.5	4	-246.0	
				-77.4
Bis-(N(NO_2)TNE)-Cubane				
Cubane	129.0	1	129.0	
C-(C_3)(H)	-1.9	-2	3.8	
C-(C_3)(N)	-3.2	2	-6.4	
N-(NO_2)(C_2)	17.8	2	35.6	
C-(N)(C)(H_2)	-6.6	2	-13.2	
C-((NO_2)$_3$)(C)	-24.9	2	-49.8	
				99.0
Tetrakis-(N(NO_2)TNE)-Cubane				
Cubane	129.0	1	129.0	
C-(C_3)(H)	-1.9	-4	7.6	
C-(C_3)(N)	-3.2	4	-12.8	
N-(NO_2)(C_2)	17.8	4	71.2	
C-(N)(C)(H_2)	-6.6	4	-26.4	
C-((NO_2)$_3$)(C)	-24.9	4	-99.6	
				69.0
Cube(CO_2TNE)$_2$				
Cubane	129.0	1	129.0	
C-(C_2)(H)	-1.9	-2	3.8	
CO(C)(O)	-35.1	2	-70.2	
O(C)(CO)	-43.1	2	-86.2	
C(O)(H_2)(C)	-8.1	2	-16.2	
C((NO_2)$_3$)(C)	-24.9	2	-49.8	
				-89.6
Cube(CO_2TNE)$_4$				
Cubane	129.0	1	129.0	
C-(C_3)(H)	-1.9	-4	7.6	
CO(C)(O)	-35.1	4	-140.4	
O(C)(CO)	-43.1	4	-172.4	
C(O)(H_2)(C)	-8.1	4	-32.4	
C((NO_2)$_3$)(C)	-24.9	4	-99.6	
				-308.2

Cube($CONHTNE)_4$				
Cubane	129.0	1	129.0	
$C-(C_3)(H)$	-1.9	-4	7.6	
$CO(C)(N)$	-32.8	4	-131.2	
$N(C)(CO)(H)$	-4.4	4	-17.6	
$C(N)(H_2)(C)$	-6.6	4	-26.4	
$C((NO_2)_3)(C)$	-24.9	4	-99.6	
				-138.2
Cube($CONH-FDNE)_4$				
Cubane	129.0	1	129.0	
$C-(C_3)(H)$	-1.9	-4	7.6	
$CO(C)(N)$	-32.8	4	-131.2	
$N(C)(CO)(H)$	-4.4	4	-17.6	
$C(N)(H_2)(C)$	-6.6	4	-26.4	
$C-(F)((NO_2)_2)(C)$	-61.5	4	-246.0	
				-284.6
Cube($CO_2FDNE)_2$				
Cubane	129.0	1	129.0	
$C-(C_3)(H)$	-1.9	-2	3.8	
$CO(C)(O)$	-35.1	2	-70.2	
$O(C)(CO)$	-43.1	2	-86.2	
$C(O)(H_2)(C)$	-8.1	2	-16.2	
$C-(F)((NO_2)_2)(C)$	-61.5	2	-123.0	
				-162.8
Cube($CO_2FDNE)_4$				
Cubane	129.0	1	129.0	
$C-(C_3)(H)$	-1.9	-4	7.6	
$CO(C)(O)$	-35.1	4	-140.4	
$O(C)(CO)$	-43.1	4	-172.4	
$C(O)(H_2)(C)$	-8.1	4	-32.4	
$C-(F)((NO_2)_2)(C)$	-61.5	4	-246.0	
				-454.6
Cubane($C(NO_2)_3)_4$				
Cubane	129.0	1	129.0	
$C-(C_3)(H)$	-1.9	-4	7.6	
$C-(C)(C_3)$	0.5	4	2.0	
$C((NO_2)-)(C)$	-24.9	4	-99.6	
				39.0
Cubane($OClO_3)_4$				
Cubane	129.0	1	129.0	
$C-(C_3)(H)$	-1.9	-4	7.6	
$C(OClO_3)$	-2.8	4	-11.2	
				125.4
Tetracyanocubane				
Cubane	129.0	1	129.0	
$C-(C_3)(H)$	-1.9	-4	7.6	
$C(CN)(C_3)$	29.0	4	116.0	
				252.6

Hexacyanocubane				
Cubane	129.0	1	129.0	
C-(C_3)(H)	-1.9	-6	11.4	
C(CN)(C_3)	29.0	6	174.0	
				314.4
Tetraisocyanocubane				
Cubane	129.0	1	129.0	
C-(C_3)(H)	-1.9	-4	7.6	
C(CN)(C_3)	29.0	4	116.0	
Isocyanide Corr.	14.9	4	59.6	
				312.2
Hexaisocyanocubane				
Cubane	129.0	1	129.0	
C-(C_3)(H)	-1.9	-6	11.4	
C(CN)(C_3)	29.0	6	174.0	
Isocyanide Corr.	14.9	6	89.4	
				403.8
Cubane(NF_2)$_4$				
Cubane	129.0	1	129.0	
C-(C_3)(H)	-1.9	-4	7.6	
N(F_2)(C)	-7.2	4	-28.8	
				107.8
Cube(($N(NO_2)_2CO$)				
Cubane	129.0	1	129.0	
C-(C_3)(H)	-1.9	-4	7.6	
$N(NO_2)$(C)(CO)	9.4	4	37.6	
$CO(N_2)$	-30.6	2	-61.2	113.0
Cube((NNO_2)$CH_2N(NO_2)CH_2N(NO_2)$)$_2$				
Cubane	129.0	1	129.0	
C-(C_3)(H)	-1.9	-4	7.6	
$N(NO_2)(C)_2$	11.2	6	67.2	
$C(H)_2(N)_2$	-7.5	6	-45.0	
				158.8
Alternative Value for $N(NO_2)(C)_2$				
Cube((NNO_2)$CH_2N(NO_2)CH_2N(NO_2)$)$_2$				
Cubane	129.0	1	129.0	
C-(C_3)(H)	-1.9	-4	7.6	
$N(NO_2)(C)_2$	17.8	6	106.8	
$C(H)_2(N)_2$	-7.5	6	-45.0	
				198.4

Cubane($N(NO_2)$-Furazane ring-$N(NO_2)$)

Cubane	129.0	1	129.0	
$C-(C_3)(H)$	-1.9	-4	7.6	
$N(NO_2)(C)_2$	17.8	4	71.2	
C(N)(C)(N-imino)	0.0	4	0.0	
N-imino(C)(O)	0.0	4		
$O(N)_2$	0.0	2		
				0.0

Cubane-Tetrakis($NHNH_2$)

Cubane	129.0	1	129.0	
$C-(C_3)(H)$	-1.9	-4	7.6	
N(N)(C)(H)	20.9	4	83.6	
$N(N)(H)_2$	11.4	4	45.6	
				265.8

Tetra($N(NO_2)_2$)cubane

Cubane	129.0	1	129.0	
$C-(C_3)(H)$	-1.9	-4	7.6	
$C-(C_3)(N)$	-3.2	4	-12.8	
$N-(NO_2)_2(C)$	20.0	4	80.0	
				203.8

Cubane-Tetrakis(CH_2NHNH_2)

Cubane	129.0	1	129.0	
$C-(C_3)(H)$	-1.9	-4	7.6	
$C-(C)(N)(H)_2$	-6.6	4	-26.4	
N(N)(C)(H)	20.9	4	83.6	
$N(N)(H)_2$	11.4	4	45.6	
				239.4

Cubane-($NH(C=NNO_2)$-NH)

Cubane	129.0	1	129.0	
$C-(C_3)(H)$	-1.9	-2	3.8	
Nitroguanidine	-21.7	1	-21.7	
$N(H_2)(C)$	4.8	-2	-9.6	
$C-(C_3)(N)$	-3.2	2	-6.4	
$N(C_2)(H)$	15.4	2	30.8	
				125.9

Appendix B

CALCULATED DENSITIES OF CUBANES

Cubane Calculated Densities

Holden Cubane Densities

Dinitrocubane

Density = (Measured)	1.660
Holden Calc =	1.700
Stine Calc =	1.736

Trinitrocubane

1,3,8	1.742
1,2,7	1.748
1,2,3	1.706
Average =	1.732
Holden Calc =	1.804
Stine Calc =	1.842
Stine + Holden % of Ave =	95.0%

Tetranitrocubane

1,3,6,8	1.738
1,2,7,8	1.853
1,2,3,4	1.799
1,2,3,6	1.795
1,2,3,8	1.771
1,2,3,5	1.725
Average =	1.780
Holden Calc =	1.882
Stine Calc =	1.922
Stine + Holden	

Density Calculated by Holden's Method

Dinitrocubane

#C	#H	#N	#O	#F	Mol. Weight
8	6.0	2	4	0	194.1

Group	Value	Number	Sub Total
C(4)	7.4	8	59.2
C-H	3.4	6	20.4
NO2	21.8	2	43.6
Non ArH Rings	-3.0	3	-9
		Sum =	114.2
		Density (Calc) =	1.70

Trinitrocubane

#C	#H	#N	#O	#F	Mol. Weight
8	5.0	3	6	0	239.1

Group	Value	Number	Sub Total
C(4)	7.4	8	59.2
C-H	3.4	5	17
NO2	21.8	3	65.4
Non ArH Rings	-3.0	3	-9
		Sum =	132.6
		Density (Calc) =	1.80

Tetranitrocubane

#C	#H	#N	#O	#F	Mol. Weight
8	4.0	4	8	0	284.1

Group	Value	Number	Sub Total
C(4)	7.4	8	59.2
C-H	3.4	4	13.6
NO2	21.8	4	87.2
Non ArH Rings	-3.0	3	-9
		Sum =	151
		Density (Calc) =	1.88

Density Calculated by Stine's Method(Linear)

Dinitrocubane

Group	Value	Number	Sub Total
C(1,-1,-1,-1)	9.755	8	78.04
C-H	5.981	6	35.89
NO2	35.88	2	71.76
		Sum =	185.69
		Density (Calc	1.74

Trinitrocubane

Group	Value	Number	Sub Total
C(1,-1,-1,-1)	9.755	8	78.04
C-H	5.981	5	29.91
NO2	35.88	3	107.64
		Sum =	215.59
		Density (Calc) =	1.84

Tetranitrocubane

Group	Value	Number	Sub Total
C(1,-1,-1,-1)	9.755	8	78.04
C-H	5.981	4	23.92
NO2	35.88	4	143.52
		Sum =	245.48
		Density (Calc) =	1.92

Cubane Calculated Densities

% of Ave =	93.6%

Pentanitrocubane		**#C**	**#H**	**#N**	**#O**	**#F**	**Mol. Weight**
1,2,3,5,6	1.830	8	3.0	5	10	0	329.1
1,2,3,4,5	1.833						
1,2,3,6,8	1.803						
Average =	1.822						
Holden Calc =	1.943						
Stine Calc =	1.984						
Stine + Holden							
% of Ave =	92.8%						

Group	**Value**	**Number**	**Sub Total**
C(4)	7.4	8	59.2
C-H	3.4	3	10.2
NO2	21.8	5	109
Non ArH Rings	-3.0	3	-9
		Sum =	169.4
		Density (Calc) =	1.94

Hexanitrocubane		**#C**	**#H**	**#N**	**#O**	**#F**	**Mol. Weight**
1,2,3,5,7,8	1.935	8	2.0	6	12	0	374.1
1,2,3,4,5,6	1.900						
1,2,3,5,6,8	1.818						
Average =	1.884						
Holden Calc =	2.058						
Stine Calc =	2.035						
Stine + Holden							
% of Ave =	92.1%						

Group	**Value**	**Number**	**Sub Total**
C(4)	7.4	8	59.2
C-H	3.4	2	6.8
NO2	21.8	6	130.8
Non ArH Rings	-3.0	5	-15
		Sum =	181.8
		Density (Calc) =	2.06

Heptanitrocubane		**#C**	**#H**	**#N**	**#O**	**#F**	**Mol. Weight**
	1.917	8	1.0	7	14	0	419.1
Holden Calc =	2.033						
Stine Calc =	2.076						
Stine + Holden							
% of Ave =	93.3%						

Group	**Value**	**Number**	**Sub Total**
C(4)	7.4	8	59.2
C-H	3.4	1	3.4
NO2	21.8	7	152.6
Non ArH Rings	-3.0	3	-9
		Sum =	206.2
		Density (Calc) =	2.03

Pentanitrocubane

Group	**Value**	**Number**	**Sub Total**
C(1,-1,-1,-1)	9.755	8	78.04
C-H	5.981	3	17.94
NO2	35.88	5	179.40
		Sum =	275.38
		Density (Calc) =	1.98

Hexanitrocubane

Group	**Value**	**Number**	**Sub Total**
C(1,-1,-1,-1)	9.755	8	78.04
C-H	5.981	2	11.96
NO2	35.88	6	215.28
		Sum =	305.28
		Density (Calc) =	2.03

Heptanitrocubane

Group	**Value**	**Number**	**Sub Total**
C(1,-1,-1,-1)	9.755	8	78.04
C-H	5.981	1	5.98
NO2	35.88	7	251.16
		Sum =	335.18
		Density (Calc) =	2.08

Cubane Calculated Densities

Octanitrocubane 1.991

#C	#H	#N	#O	#F	Mol. Weight
8	0.0	8	16	0	464.1

Holden Calc = 2.066
Stine Calc = 2.111
Stine + Holden % of Ave = 95.3%

Group	Value	Number	Sub Total
C(4)	7.4	8	59.2
C-H	3.4	0	0
NO2	21.8	8	174.4
Non ArH Rings	-3.0	3	-9
		Sum =	224.6
		Density (Calc) =	2.07

Cubanedinitrate

#C	#H	#N	#O	#F	Mol.Weight
8	6	2	6	0	226.1

Holden Calc = 1.854
Stine Calc = 1.788

Average = 1.821
92.2% of Ave= 1.679

Group	Value	Number	Sub Total
C(4)	7.4	8	59.2
C-H	3.4	6	20.4
O(2)	6.9	2	13.8
NO2	21.8	2	43.6
Non ArH Rings	-3.0	5	-15
		Sum =	122
		Density (Calc) =	1.85

Cubanetrinitrate

#C	#H	#N	#O	#F	Mol. Weight
8	5	3	9	0	287.1

Holden Calc = 1.873
Stine Calc = 1.891

Average = 1.882
92.2% of Ave= 1.735

Group	Value	Number	Sub Total
C(4)	7.4	8	59.2
C-H	3.4	5	17
O(2)	6.9	3	20.7
NO2	21.8	3	65.4
Non ArH Rings	-3.0	3	-9
		Sum =	153.3
		Density (Calc) =	1.87

Octanitrocubane

Group	Value	Number	Sub Total
C(1,-1,-1,-1)	9.755	8	78.04
C-H	5.981	0	0.00
NO2	35.88	8	287.04
		Sum =	365.08
		Density (Calc) =	2.11

Cubanedinitrate

Group	Value	Number	Sub Total
C(1,-1,-1,-1)	9.755	8	78.04
C-H	5.981	6	35.89
O(1,1)	12.18	2	24.36
NO2	35.88	2	71.76
		Sum =	210.04
		Density (Calc) =	1.79

Cubanetrinitrate

Group	Value	Number	Sub Total
C(1,-1,-1,-1)	9.755	8	78.04
C-H	5.981	5	29.91
O(1,1)	12.18	3	36.53
NO2	35.88	3	107.64
		Sum =	252.12
		Density (Calc) =	1.89

Cubane Calculated Densities

Cubanetetranitrate

Holden Calc =	1.949
Stine Calc =	1.965
Average =	1.957
92.2% of Ave=	1.804

#C	#H	#N	#O	#F	Mol. Weight
8	4.0	4	12	0	348.1

Group	Value	Number	Sub Total
C(4)	7.4	8	59.2
C-H	3.4	4	13.6
O(2)	6.9	4	27.6
NO2	21.8	4	87.2
Non ArH Rings	-3.0	3	-9
		Sum =	178.6
		Density (Calc) =	1.95

Cubanepentanitrate

Holden Calc =	2.067
Stine Calc =	2.020
Average =	2.044
92.2% of Ave=	1.884

#C	#H	#N	#O	#F	Mol. Weight
8	3	5	15	0	409.1

Group	Value	Number	Sub Total
C(4)	7.4	8	59.2
C-H	3.4	3	10.2
O(2)	6.9	5	34.5
NO2	21.8	5	109
Non ArH Rings	-3.0	5	-15
		Sum =	197.9
		Density (Calc) =	2.07

Cubanehexanitrate

Holden Calc =	2.051
Stine Calc =	2.063
Average =	2.057
92.2% of Ave=	1.897

#C	#H	#N	#O	#F	Mol. Weight
8	2	6	18	0	470.1

Group	Value	Number	Sub Total
C(4)	7.4	8	59.2
C-H	3.4	2	6.8
O(2)	6.9	6	41.4
NO2	21.8	6	130.8
Non ArH Rings	-3.0	3	-9
		Sum =	229.2
		Density (Calc) =	2.05

Cubanetetranitrate

Group	Value	Number	Sub Total
C(1,-1,-1,-1)	9.755	8	78.04
C-H	5.981	4	23.92
O(1,1)	12.18	4	48.71
NO2	35.88	4	143.52
		Sum =	294.20
		Density (Calc) =	1.96

Cubanepentanitrate

Group	Value	Number	Sub Total
C(1,-1,-1,-1)	9.755	8	78.04
C-H	5.981	3	17.94
O(1,1)	12.18	5	60.89
NO2	35.88	5	179.40
		Sum =	336.27
		Density (Calc) =	2.02

Cubanehexanitrate

Group	Value	Number	Sub Total
C(1,-1,-1,-1)	9.755	8	78.04
C-H	5.981	2	11.96
O(1,1)	12.18	6	73.07
NO2	35.88	6	215.28
		Sum =	378.35
		Density (Calc) =	2.06

Cubane-1,2-(bis-N-nitropropellane)

		#C	#H	#N	#O	#F	Mol. Weight
Holden Calc =	1.787	9	6	4	5	0	250.2
Stine Calc =	1.969						
Average =	1.878						

Group	Value	Number	Sub Total
C(4)	7.4	8	59.2
C(3)	8.1	1	8.1
C-H	3.4	6	20.4
O(1)	6.9	1	6.9
NO2	21.8	2	43.6
N(3)	6.9	2	13.8
Non ArH Rings	-3.0	4	-12
		Sum =	140
		Density (Calc) =	1.79

Cubane-1,2-(bis-N-nitropropellane)

Group	Value	Number	Sub Total
C(1,-1,-1,-1)	9.755	6	58.53
C(-1,-1,-1,-1	9.673	2	19.35
C(-1,-1,2)	12.65	1	12.65
C-H	5.981	6	35.89
O(2)	12.75	1	12.75
NO2	35.88	2	71.76
		Sum =	210.93
		Density (Calc) =	1.97

Cubane-Bis-(bis-N-nitropropellane)

		#C	#H	#N	#O	#F	Mol. Weight
Holden Calc =	1.899	10	4	8	10	0	396.2
Stine Calc =	2.222						
Average =	2.061						

Group	Value	Number	Sub Total
C(4)	7.4	8	59.2
C(3)	8.1	2	16.2
C-H	3.4	4	13.6
O(1)	6.9	2	13.8
N(3)	6.9	4	27.6
NO2	21.8	4	87.2
Non ArH Rings	-3.0	3	-9
		Sum =	208.6
		Density (Calc) =	1.90

Cubane-Bis-(bis-N-nitropropellane)

Group	Value	Number	Sub Total
C(1,-1,-1,-1)	9.755	4	39.02
C(-1,-1,-1,-1	9.673	4	38.69
C(-1,-1,2)	12.65	2	25.31
C-H	5.981	4	23.92
O(2)	12.75	2	25.51
NO2	35.88	4	143.52
		Sum =	295.97
		Density (Calc) =	2.22

Cubane Calculated Densities

Bis-(N(NO2)FDNE) Cubane

Density =	1.827	#C	#H	#N	#O	#F	Mol. Weight
Measured		12	10	8	12	2	496.3

		Group	Value	Number	Sub Total
Holden Calc =	1.799	C(4)	7.4	12	88.8
Stine Calc =	1.839	C-H	3.4	10	34
Average =	1.819	N(3)	6.9	2	13.8
		C-F	8.7	2	17.4
		NO2	21.8	6	130.8
		Non ArH Rings	-3.0	3	-9
				Sum =	275.8
				Density (Calc) =	1.80

Bis-N(NO2)TNE)Cubane

	#C	#H	#N	#O	#F	Mol. Weight
	12	10	10	16	0	550.3

		Group	Value	Number	Sub Total
Holden Calc =	1.822	C(4)	7.4	12	88.8
Stine Calc =	1.849	C-H	3.4	10	34
Average =	1.836	N(3)	6.9	2	13.8
		NO2	21.8	8	174.4
		Non ArH Rings	-3.0	3	-9
				Sum =	302
				Density (Calc) =	1.82

Bis-1,4-(N(NO2)FDNE) Cubane

Group	Value	Number	Sub Total
C(1,-1,-1,-1)	9.755	8	78.04
C(1,1,1,1)	9.673	4	38.69
F	12.93	2	25.86
C-H	5.981	12	71.77
NO2	35.88	6	215.28
N(1,1,1)	9.234	2	18.47
		Sum =	448.11
		Density (Calc) =	1.84

Bis-1,4-(N(NO2)FDNE) Cubane

Group	Value	Number	Sub Total
C(1,-1,-1,-1)	9.755	8	78.04
C(1,1,1,1)	9.673	4	38.69
C-H	5.981	12	71.77
NO2	35.88	8	287.04
N(1,1,1)	9.234	2	18.47
		Sum =	494.01
		Density (Calc) =	1.85

Cubane Calculated Densities

Tetrakis-(N(NO2)TNE) Cubane

#C	#H	#N	#O	#F	Mol. Weight
16	12	20	32	0	996.4

Holden Calc =	1.892
Stine Calc =	1.974
Average =	1.933

Group	Value	Number	Sub Total
C(4)	7.4	16	118.4
C-H	3.4	12	40.8
N(3)	6.9	4	27.6
NO2	21.8	16	348.8
Non ArH Rings	-3.0	3	-9
		Sum =	526.6
		Density (Calc) =	1.89

Tetrakis-(N(NO2)TNE) Cubane

Group	Value	Number	Sub Total
C(1,-1,-1,-1)	9.755	8	78.04
C(1,1,1,1)	9.673	8	77.38
C-H	5.981	12	71.77
NO2	35.88	16	574.08
N(1,1,1)	9.234	4	36.94
		Sum =	838.21
		Density (Calc) =	1.97

Tetrakis-(N(NO2)FDNE) Cubane

#C	#H	#N	#O	#F	Mol. Weight
16	14	16	24	4	890.4

Holden Calc =	1.851
Stine Calc =	1.949
Average =	1.900

Group	Value	Number	Sub Total
C(4)	7.4	16	118.4
C-H	3.4	14	47.6
N(3)	6.9	4	27.6
C-F	8.7	4	34.8
NO2	21.8	12	261.6
Non ArH Rings	-3.0	3	-9
		Sum =	481
		Density (Calc) =	1.85

Tetrakis-(N(NO2)FDNE) Cubane

Group	Value	Number	Sub Total
C(1,-1,-1,-1)	9.755	8	78.04
C(1,1,1,1)	9.673	8	77.38
F	12.93	4	51.72
C-H	5.981	14	83.73
NO2	35.88	12	430.56
N(1,1,1)	9.234	4	36.94
		Sum =	758.37
		Density (Calc) =	1.95

Cubane Calculated Densities

Bis-(N(NO2)H) Cubane

	#C	#H	#N	#O	#F	Mol. Weight
Density = 1.690	8	8	4	4	0	224.2
Measured						
Holden Calc = 1.678						
Stine Calc = 1.735						
Average = 1.706						

Group	Value	Number	Sub Total
C(4)	7.4	8	59.2
C-H	3.4	6	20.4
N(3)	6.9	2	13.8
NO2	21.8	2	43.6
N-H	2.8	2	5.6
Non ArH Rings	-3.0	3	-9
		Sum =	133.6
		Density (Calc) =	1.68

Bis-(N(NO2)H) Cubane

Group	Value	Number	Sub Total
C(1,-1,-1,-1)	9.755	8	78.04
N-H	5.199	2	10.40
C-H	5.981	6	35.89
NO2	35.88	2	71.76
N(1,1,1)	9.234	2	18.47
		Sum =	214.55
		Density (Calc) =	1.73

Tetrakis-(N(NO2)H) Cubane

	#C	#H	#N	#O	#F	Mol. Weight
	8	8	8	8	0	344.2
Holden Calc = 1.813						
Stine Calc = 1.885						
Average = 1.849						

Group	Value	Number	Sub Total
C(4)	7.4	8	59.2
C-H	3.4	4	13.6
N(3)	6.9	4	27.6
NO2	21.8	4	87.2
N-H	2.8	4	11.2
Non ArH Rings	-3.0	3	-9
		Sum =	189.8
		Density (Calc) =	1.81

Tetrakis-(N(NO2)H) Cubane

Group	Value	Number	Sub Total
C(1,-1,-1,-1)	9.755	8	78.04
N-H	5.199	4	20.80
C-H	5.981	4	23.92
NO2	35.88	4	143.52
N(1,1,1)	9.234	4	36.94
		Sum =	303.22
		Density (Calc) =	1.88

Cubane Calculated Densities

Bis-(N(NO2)2)-Cubane

#C	#H	#N	#O	#F	Mol. Weight
8	6	6	8	0	314.2

Holden Calc =	1.831
Stine Calc =	1.891
Average =	1.861

Group	Value	Number	Sub Total
C(4)	7.4	8	59.2
C-H	3.4	6	20.4
N(3)	6.9	2	13.8
NO2	21.8	4	87.2
N-H	2.8	0	0
Non ArH Rings	-3.0	3	-9
		Sum =	171.6
		Density (Calc) =	1.83

Bis-(N(NO2)2)-Cubane

Group	Value	Number	Sub Total
C(1,-1,-1,-1)	9.755	8	78.04
N-H	5.199	0	0.00
C-H	5.981	6	35.89
NO2	35.88	4	143.52
N(1,1,1)	9.234	2	18.47
		Sum =	275.91
		Density (Calc) =	1.89

Tetrakis-(N(NO2)2)-Cubane

#C	#H	#N	#O	#F	Mol. Weight
8	4	12	16	0	524.2

Holden Calc =	1.972
Stine Calc =	2.043
Average =	2.008

Group	Value	Number	Sub Total
C(4)	7.4	8	59.2
C-H	3.4	4	13.6
N(3)	6.9	4	27.6
NO2	21.8	8	174.4
N-H	2.8	0	0
Non ArH Rings	-3.0	3	-9
		Sum =	265.8
		Density (Calc) =	1.97

Tetrakis-(N(NO2)2)-Cubane

Group	Value	Number	Sub Total
C(1,-1,-1,-1)	9.755	8	78.04
N-H	5.199	0	0.00
C-H	5.981	4	23.92
NO2	35.88	8	287.04
N(1,1,1)	9.234	4	36.94
		Sum =	425.94
		Density (Calc) =	2.04

Cubane Calculated Densities

Bis-Trinitromethylcubane

#C	#H	#N	#O	#F	Mol. Weight
10	6	6	12	0	402.2

		Group	Value	Number	Sub Total
		C(4)	7.4	10	74
Holden Calc =	1.860	C-H	3.4	6	20.4
Stine Calc =	1.916	NO2	21.8	6	130.8
		Non ArH Rings	-3.0	3	-9
Average =	1.888			Sum =	216.2
				Density (Calc) =	1.86

Bis-Trinitromethylcubane

Group	Value	Number	Sub Total
C(1,-1,-1,-1)	9.755	8	78.04
C(1,1,1,1)	9.673	2	19.35
C-H	5.981	6	35.89
NO2	35.88	6	215.28
		Sum =	348.55
		Density (Calc) =	1.92

Tetrakis-Trinitromethylcubane

#C	#H	#N	#O	#F	Mol. Weight
12	4	12	24	0	700.2

		Group	Value	Number	Sub Total
Holden Calc =	1.972	C(4)	7.4	12	88.8
Stine Calc =	2.035	C-H	3.4	4	13.6
Average =	2.004	NO2	21.8	12	261.6
		Non ArH Rings	-3.0	3	-9
				Sum =	355
				Density (Calc) =	1.97

Tetrakis-Trinitromethylcubane

Group	Value	Number	Sub Total
C(1,-1,-1,-1)	9.755	8	78.04
C(1,1,1,1)	9.673	4	38.69
C-H	5.981	4	23.92
NO2	35.88	12	430.56
		Sum =	571.22
		Density (Calc) =	2.04

Tetracyanocubane

#C	#H	#N	#O	#F	Mol. Weight
12	4	4	0	0	204.2

		Group	Value	Number	Sub Total
Holden Calc =	1.473	C(4)	7.4	8	59.2
Stine Calc =	1.470	C(2)	11.5	4	46
Average =	1.471	C-H	3.4	4	13.6
		N(1)	7.2	4	28.8
		Non ArH Rings	-3.0	3	-9
				Sum =	138.6
				Density (Calc) =	1.47

Group	Value	Number	Sub Total
C(1,-1,-1,-1)	9.755	8	78.04
C(3,1)	16.58	4	66.32
C-H	5.981	4	23.92
N(3)	15.6	4	62.40
		Sum =	230.68
		Density (Calc) =	1.47

Cubane Calculated Densities

Cubane-Bis-Trinitroethylester

#C	#H	#N	#O	#F	Mol. Weight
14	10	6	16	0	518.3

		Group	Value	Number	Sub Total
Holden Calc =	1.785	C(4)	7.4	12	88.8
Stine Calc =	1.832	C(3)	8.1	2	16.2
Average =	1.808	C-H	3.4	10	34
		O(1)	7.9	2	15.8
		O(2)	6.9	2	13.8
		NO2	21.8	6	130.8
		Non ArH Rings	-3.0	3	-9
				Sum =	290.4
				Density (Calc) =	1.78

Cubane-Tetrakis-Trinitroethylester

#C	#H	#N	#O	#F	Mol. Weight
20	12	12	32	0	932.4

		Group	Value	Number	Sub Total
Holden Calc =	1.852	C(4)	7.4	16	118.4
Stine Calc =	1.903	C(3)	8.1	4	32.4
Average =	1.878	C-H	3.4	12	40.8
		O(1)	7.9	4	31.6
		O(2)	6.9	4	27.6
		NO2	21.8	12	261.6
		Non ArH Rings	-3.0	3	-9
				Sum =	503.4
				Density (Calc) =	1.85

Cubane-Bis-Trinitroethylester

Group	Value	Number	Sub Total
C(1,-1,-1,-1)	9.755	8	78.04
C(1,1,1,1)	9.673	4	38.69
C(2,1,1)	14.57	2	29.13
C-H	5.981	10	59.81
NO2	35.880	6	215.28
O(1,1)	12.178	2	24.36
O(2)	12.172	2	24.34
		Sum =	469.65
		Density (Calc) =	1.83

Cubane-Tetrakis-Trinitroethylester

Group	Value	Number	Sub Total
C(1,-1,-1,-1)	9.755	8	78.04
C(1,1,1,1)	9.673	8	77.38
C(2,1,1)	14.57	4	58.26
C-H	5.981	12	71.77
NO2	35.880	12	430.56
O(1,1)	12.178	4	48.71
O(2)	12.172	4	48.69
		Sum =	813.42
		Density (Calc) =	1.90

Cubane Calculated Densities

Cubane-Bis-Fluorodinitroethylester

#C	#H	#N	#O	#F	Mol. Weight
14	10	4	12	2	464.2

Holden Calc =	1.757
Stine Calc =	1.819
Average =	1.788

Group	Value	Number	Sub Total
C(4)	7.4	12	88.8
C(3)	8.1	2	16.2
C-H	3.4	10	34
O(1)	7.9	2	15.8
O(2)	6.9	2	13.8
F	8.7	2	17.4
NO2	21.8	4	87.2
Non ArH Rings	-3.0	3	-9
		Sum =	264.2
		Density (Calc) =	1.76

Cubane-Tetrakis-Fluorodinitroethylester

Density =	1.762
X-Ray	

#C	#H	#N	#O	#F	Mol. Weight
20	12	8	24	4	824.3

Holden Calc =	1.828
Stine Calc =	1.897
Average =	1.862

Group	Value	Number	Sub Total
C(4)	7.4	16	118.4
C(3)	8.1	4	32.4
C-H	3.4	12	40.8
O(1)	7.9	4	31.6
O(2)	6.9	4	27.6
F	8.7	4	34.8
NO2	21.8	8	174.4
Non ArH Rings	-3.0	3	-9
		Sum =	451
		Density (Calc) =	1.83

Cubane-Bis-Fluorodinitroethylester

Group	Value	Number	Sub Total
C(1,-1,-1,-1)	9.755	8	78.04
C(1,1,1,1)	9.673	4	38.69
C(2,1,1)	14.57	2	29.13
C-H	5.981	10	59.81
NO2	35.880	4	143.52
O(1,1)	12.178	2	24.36
O(2)	12.172	2	24.34
F	12.929	2	25.86
		Sum =	423.75
		Density (Calc) =	1.82

Cubane-Tetrakis-Fluorodinitroethylester

Group	Value	Number	Sub Total
C(1,-1,-1,-1)	9.755	8	78.04
C(1,1,1,1)	9.673	8	77.38
C(2,1,1)	14.57	4	58.26
C-H	5.981	12	71.77
NO2	35.880	8	287.04
O(1,1)	12.178	4	48.71
O(2)	12.172	4	48.69
F	12.929	4	51.72
		Sum =	721.61
		Density (Calc) =	1.90

Cubane Calculated Densities

Cubane-Tetrakis-Fluorodinitroethylamide

Density =	1.762	#C	#H	#N	#O	#F	Mol. Weight
X-Ray		20	16	12	20	4	820.4

		Group	Value	Number	Sub Total
Holden Calc =	1.802	C(4)	7.4	16	118.4
Stine Calc =	1.856	C(3)	8.1	4	32.4
Average =	1.829	C-H	3.4	16	54.4
		O(1)	7.9	4	31.6
		N(3)	4.6	4	18.4
		F	8.7	4	34.8
		NO2	21.8	8	174.4
		Non ArH Rings	-3.0	3	-9
				Sum =	455.4
				Density (Calc) =	1.80

Cubane-Tetrakis-Trinitroethylamide

	#C	#H	#N	#O	#F	Mol. Weight
	20	16	16	28	0	928.4

		Group	Value	Number	Sub Total
Holden Calc =	1.828	C(4)	7.4	16	118.4
Stine Calc =	1.867	C(3)	8.1	4	32.4
Average =	1.848	C-H	3.4	16	54.4
		O(1)	7.9	4	31.6
		N(3)	4.6	4	18.4
		NO2	21.8	12	261.6
		Non ArH Rings	-3.0	3	-9
				Sum =	507.8
				Density (Calc) =	1.83

Cubane-Tetrakis-Fluorodinitroethylamide

Group	Value	Number	Sub Total
C(1,-1,-1,-1)	9.755	8	78.04
C(1,1,1,1)	9.673	8	77.38
C(2,1,1)	14.57	4	58.26
C-H	5.981	16	95.70
NO2	35.880	8	287.04
O(1,1)	12.178	4	48.71
N(3)	9.234	4	36.94
F	12.929	4	51.72
		Sum =	733.78
		Density (Calc) =	1.86

Cubane-Tetrakis-Trinitroethylamide

Group	Value	Number	Sub Total
C(1,-1,-1,-1)	9.755	8	78.04
C(1,1,1,1)	9.673	8	77.38
C(2,1,1)	14.57	4	58.26
C-H	5.981	16	95.70
NO2	35.880	12	430.56
N(1,1,1)	9.234	4	36.94
O(2)	12.172	4	48.69
		Sum =	825.56
		Density (Calc	1.87

Cubane Calculated Densities

Cubane(N(NO2)CH2N(NO2)CH2N(NO2))2

#C	#H	#N	#O	#F	Mol. Weight
12	12	12	12	0	516.3

Holden Calc = 1.851
Stine Calc = 1.867
Average = 1.859

Group	Value	Number	Sub Total
C(4)	7.4	12	88.8
C-H	3.4	12	40.8
N(3)	4.6	6	27.6
NO2	21.8	6	130.8
Non ArH Rings	-3.0	3	-9
		Sum =	279
		Density (Calc) =	1.85

Cubane-bis(NHNH2)

#C	#H	#N	#O	#F	Mol. Weight
8	12	4	0	0	164.2

Holden Calc = 1.552
Stine Calc = 1.498
Average = 1.525

Group	Value	Number	Sub Total
C(4)	7.4	8	59.2
C-H	3.4	6	20.4
N-H	2.8	6	16.8
N(3)	4.6	4	18.4
Non ArH Rings	-3.0	3	-9
		Sum =	105.8
		Density (Calc) =	1.55

Cubane-Tetrakis(NHNH2)

#C	#H	#N	#O	#F	Mol. Weight
8	16	8	0	0	224.3

Holden Calc = 1.671
Stine Calc = 1.563
Average = 1.617

Group	Value	Number	Sub Total
C(4)	7.4	8	59.2
C-H	3.4	4	13.6
N-H	2.8	12	33.6
N(3)	4.6	8	36.8
Non ArH Rings	-3.0	3	-9
		Sum =	134.2
		Density (Calc) =	1.67

Cubane(N(NO2)CH2N(NO2)CH2N(NO2))2

Group	Value	Number	Sub Total
C(1,-1,-1,-1)	9.755	8	78.04
C(1,1,1,1)	9.673	4	38.69
N(1,1,1)	9.234	6	55.404
C-H	5.981	12	71.77
NO2	35.880	6	215.28
		Sum =	459.19
		Density (Calc) =	1.87

Cubane-bis(NHNH2)

Group	Value	Number	Sub Total
C(1,-1,-1,-1)	9.755	8	78.04
C-H	5.981	6	35.89
N(1,1,1)	9.234	4	36.94
N-H	5.199	6	31.19
		Sum =	182.06
		Density (Calc) =	1.50

Cubane-Tetrakis(NHNH2)

Group	Value	Number	Sub Total
C(1,-1,-1,-1)	9.755	8	78.04
C-H	5.981	4	23.92
N(1,1,1)	9.234	8	73.87
N-H	5.199	12	62.39
		Sum =	238.22
		Density (Calc) =	1.56

Cubane Calculated Densities

Cubane-Tetrakis(NF2)

#C	#H	#N	#O	#F	Mol. Weight
8	4	4	0	8	308.1

Holden Calc = 2.030
Stine Calc = 2.111
Average = 2.070

Group	Value	Number	Sub Total
C(4)	7.4	8	59.2
C-H	3.4	4	13.6
N-F	8.7	8	69.6
N(3)	4.6	4	18.4
Non ArH Rings	-3.0	3	-9
		Sum =	151.8
		Density (Calc) =	2.03

Cubane-Tetrakis(NF2)

Group	Value	Number	Sub Total
C(1,-1,-1,-1)	9.755	8	78.04
C-H	5.981	4	23.92
N(1,1,1)	9.234	4	36.94
N-H	12.929	8	103.43
		Sum =	242.33
		Density (Calc) =	2.11

Cubane-Tetrakis(NHNH3ClO4)

#C	#H	#N	#O	#Cl	Mol. Weight
8	20	8	16	4	626.3

Holden Calc = 2.062
Stine Calc = #VALUE!
Average = #VALUE!

Group	Value	Number	Sub Total
C(4)	7.4	8	59.2
C-H	3.4	4	13.6
N-H	2.8	16	44.8
N(4)	3.5	4	14
O(2)	6.9	12	82.8
O(1)	7.9	4	31.6
Cl(4)	12.1	4	48.4
N(3)	4.6	4	18.4
Non ArH Rings	-3.0	3	-9
		Sum =	303.8
		Density (Calc) =	2.06

Cubane-Tetrakis(NHNH3ClO4)

Group	Value	Number	Sub Total
C(1,-1,-1,-1)	9.755	8	78.04
C-H	5.981	4	23.92
N(1,1,1,1)	5.981	4	23.92
O(1)	12.75	4	51.02
O(2)	12.178	12	146.14
N(1,1,1)	9.234	4	36.94
N-H	5.199	16	83.18
(2,2,2,1)	??	16	#VALUE!
		Sum =	#VALUE!
		Density (Calc) =	#VALUE!

Cubane Calculated Densities

Cubane-(NH(C=NNO2)-NH)

#C	#H	#N	#O	#Cl	Mol. Weight
9	8	4	2	0	204.2

Holden Calc = 1.762
Stine Calc = 1.755
Average = 1.758

Group	Value	Number	Sub Total
C(4)	7.4	8	59.2
C-H	3.4	6	20.4
N-H	2.8	2	5.6
NO2	21.8	1	21.8
N(2)	8.7	1	8.7
N(3)	4.6	2	9.2
Non ArH Rings	-3.0	3	-9
		Sum =	115.9
		Density (Calc) =	1.76

Cubane-(NH(C=NNO2)-NH)

Group	Value	Number	Sub Total
C(1,-1,-1,-1)	9.755	8	78.04
C-H	5.981	6	35.89
N(2,1)	14.49	1	14.49
NO2	35.880	1	35.88
N(1,1,1)	9.234	2	18.47
N-H	5.199	2	10.40
		Sum =	193.16
		Density (Calc) =	1.76

Cubane-Tetrakis(CH2NHNH2)

#C	#H	#N	#O	#F	Mol. Weight
12	24	8	0	0	280.4

Holden Calc = 1.468
Stine Calc = 1.371
Average = 1.419

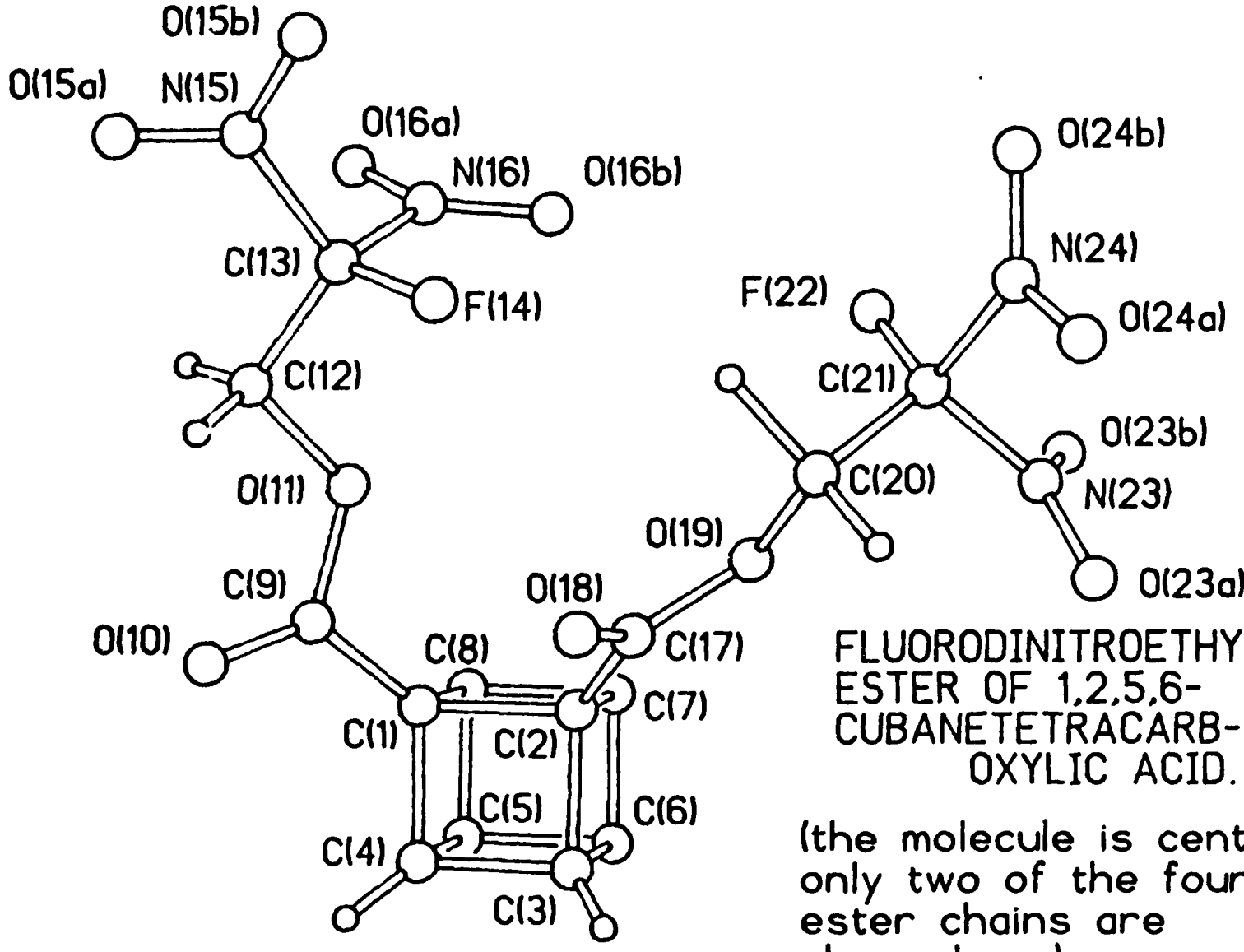
Group	Value	Number	Sub Total
C(4)	7.4	12	88.8
C-H	3.4	12	40.8
N-H	2.8	12	33.6
N(3)	4.6	8	36.8
Non ArH Rings	-3.0	3	-9
		Sum =	191
		Density (Calc) =	1.47

Cubane-Tetrakis(CH2NHNH2)

Group	Value	Number	Sub Total
C(1,-1,-1,-1)	9.755	8	78.04
C(1,1,1,1)	13.39	4	53.56
C-H	5.981	12	71.77
N(1,1,1)	9.234	8	73.87
N-H	5.199	12	62.39
		Sum =	339.63
		Density (Calc) =	1.37

Appendix C

X-RAY CRYSTAL STRUCTURES AND STRUCTURAL PARAMETERS



FLUORODINITROETHYL ESTER OF 1,2,5,6-CUBANETETRACARB-OXYLIC ACID.

(the molecule is centric; only two of the four ester chains are shown here)

Table 2. Bond lengths (Å)

C(1)-C(2)	1.574	(4)	C(1)-C(4)	1.544	(4)
C(1)-C(8)	1.572	(4)	C(1)-C(9)	1.476	(4)
C(2)-C(3)	1.564	(4)	C(2)-C(7)	1.565	(4)
C(2)-C(17)	1.487	(4)	C(3)-C(4)	1.558	(4)
C(3)-C(6)	1.572	(4)	C(4)-C(5)	1.565	(4)
C(6)-C(7)	1.544	(4)	C(9)-O(10)	1.194	(3)
C(9)-O(11)	1.343	(4)	O(11)-C(12)	1.425	(4)
C(12)-C(13)	1.478	(5)	C(13)-F(14)	1.336	(4)
C(13)-N(15)	1.517	(4)	C(13)-N(16)	1.500	(6)
N(15)-O(15A)	1.181	(4)	N(15)-O(15B)	1.173	(4)
N(16)-O(16A)	1.200	(7)	N(16)-O(16B)	1.215	(7)
C(17)-O(18)	1.192	(3)	C(17)-O(19)	1.345	(4)
O(19)-C(20)	1.443	(4)	C(20)-C(21)	1.504	(5)
C(21)-F(22)	1.319	(4)	C(21)-N(23)	1.535	(4)
C(21)-N(24)	1.535	(4)	N(23)-O(23A)	1.203	(4)
N(23)-O(23B)	1.204	(4)	N(24)-O(24A)	1.202	(4)
N(24)-O(24B)	1.198	(4)			

Table 3. Bond angles (°)

C(4)-C(1)-C(2)	90.7(2)	C(8)-C(1)-C(2)	88.7(2)
C(8)-C(1)-C(4)	90.9(2)	C(9)-C(1)-C(2)	122.6(2)
C(9)-C(1)-C(4)	126.4(2)	C(9)-C(1)-C(8)	126.4(3)
C(3)-C(2)-C(1)	88.7(2)	C(7)-C(2)-C(1)	90.7(2)
C(7)-C(2)-C(3)	90.5(2)	C(17)-C(2)-C(1)	121.2(2)
C(17)-C(2)-C(3)	124.6(3)	C(17)-C(2)-C(7)	129.6(2)
C(4)-C(3)-C(2)	90.6(2)	C(6)-C(3)-C(2)	88.8(2)
C(6)-C(3)-C(4)	91.1(2)	C(3)-C(4)-C(1)	90.0(2)
C(5)-C(4)-C(1)	89.8(2)	C(5)-C(4)-C(3)	89.5(2)
C(6)-C(5)-C(4)	90.7(2)	C(8)-C(5)-C(4)	90.5(2)
C(8)-C(5)-C(6)	88.7(2)	C(5)-C(6)-C(3)	88.7(2)
C(7)-C(6)-C(3)	90.9(2)	C(7)-C(6)-C(5)	90.7(2)
C(6)-C(7)-C(2)	89.8(2)	C(8)-C(7)-C(2)	89.5(2)
C(8)-C(7)-C(6)	90.0(2)	C(5)-C(8)-C(1)	88.8(2)
C(7)-C(8)-C(1)	91.1(2)	C(7)-C(8)-C(5)	90.6(2)
O(10)-C(9)-C(1)	126.1(3)	O(11)-C(9)-C(1)	110.5(2)
O(11)-C(9)-O(10)	123.4(3)	C(12)-O(11)-C(9)	115.8(2)
C(13)-C(12)-O(11)	106.0(3)	F(14)-C(13)-C(12)	111.4(4)
N(15)-C(13)-C(12)	112.2(3)	N(15)-C(13)-F(14)	106.9(3)
N(16)-C(13)-C(12)	114.0(3)	N(16)-C(13)-F(14)	105.4(4)
N(16)-C(13)-N(15)	106.4(3)	O(15A)-N(15)-C(13)	117.0(3)
O(15B)-N(15)-C(13)	116.8(3)	O(15B)-N(15)-O(15A)	126.2(3)
O(16A)-N(16)-C(13)	111.9(5)	O(16B)-N(16)-C(13)	116.2(6)
O(16B)-N(16)-O(16A)	131.6(6)	O(18)-C(17)-C(2)	124.6(3)
O(19)-C(17)-C(2)	112.0(2)	O(19)-C(17)-O(18)	123.3(3)
C(20)-O(19)-C(17)	113.7(2)	C(21)-C(20)-O(19)	104.0(3)
F(22)-C(21)-C(20)	113.6(3)	N(23)-C(21)-C(20)	112.4(3)
N(23)-C(21)-F(22)	106.7(3)	N(24)-C(21)-C(20)	109.2(3)
N(24)-C(21)-F(22)	108.1(3)	N(24)-C(21)-N(23)	106.5(2)
O(23A)-N(23)-C(21)	115.4(3)	O(23B)-N(23)-C(21)	117.3(3)
O(23B)-N(23)-O(23A)	127.3(3)	O(24A)-N(24)-C(21)	115.4(3)
O(24B)-N(24)-C(21)	117.1(4)	O(24B)-N(24)-O(24A)	127.5(3)

TORSION ANGLES FOR CUBANE 1,2,5,6 -TETRA -DINITROFLUORO

C4	C1	C2	C3	-0.2
C4	C1	C2	C7	90.2
C4	C1	C2	C17	-130.8
C8	C1	C2	C3	-91.2
C8	C1	C2	C7	-0.7
C8	C1	C2	C17	138.2
C9	C1	C2	C3	135.2
C9	C1	C2	C7	-134.3
C9	C1	C2	C17	4.6
C1	C2	C3	C4	0.2
C1	C2	C3	C6	91.3
C7	C2	C3	C4	-90.5
C7	C2	C3	C6	0.6
C17	C2	C3	C4	128.1
C17	C2	C3	C6	-140.8
C2	C1	C4	C3	0.2
C2	C1	C4	C5	-89.3
C8	C1	C4	C3	88.9
C8	C1	C4	C5	-0.6
C9	C1	C4	C3	-132.6
C9	C1	C4	C5	137.9
C2	C3	C4	C1	-0.2
C2	C3	C4	C5	89.5
C6	C3	C4	C1	-89.0
C6	C3	C4	C5	0.7
C1	C4	C5	C6	89.3
C1	C4	C5	C8	0.6
C3	C4	C5	C6	-0.7
C3	C4	C5	C8	-89.4
C2	C3	C6	C5	-91.3
C2	C3	C6	C7	-0.6
C4	C3	C6	C5	-0.7
C4	C3	C6	C7	90.0
C4	C5	C6	C3	0.7
C4	C5	C6	C7	-90.2
C8	C5	C6	C3	91.2
C8	C5	C6	C7	0.2
C1	C2	C7	C6	-89.3
C1	C2	C7	C8	0.7
C3	C2	C7	C6	-0.6
C3	C2	C7	C8	89.4
C17	C2	C7	C6	137.6
C17	C2	C7	C8	-132.4
C3	C6	C7	C2	0.6
C3	C6	C7	C8	-88.9
C5	C6	C7	C2	89.3
C5	C6	C7	C8	-0.2
C2	C1	C8	C5	91.3
C2	C1	C8	C7	0.7
C4	C1	C8	C5	0.6
C4	C1	C8	C7	-90.0
C9	C1	C8	C5	-137.9
C9	C1	C8	C7	131.5
C4	C5	C8	C1	-0.6
C4	C5	C8	C7	90.5

C6	C5	C8	C1	-91.3
C6	C5	C8	C7	-0.2
C2	C7	C8	C1	-0.7
C2	C7	C8	C5	-89.5
C6	C7	C8	C1	89.0
C6	C7	C8	C5	0.2
C2	C1	C9	O10	-117.8
C2	C1	C9	O11	61.0
C4	C1	C9	O10	1.7
C4	C1	C9	O11	-179.6
C8	C1	C9	O10	126.3
C8	C1	C9	O11	-55.0
C1	C9	O11	C12	-179.6
O10	C9	O11	C12	-0.9
C9	O11	C12	C13	146.1
O11	C12	C13	F14	-61.0
O11	C12	C13	N15	179.2
O11	C12	C13	N16	58.1
C12	C13	N15	O15A	-17.6
C12	C13	N15	O15B	162.1
F14	C13	N15	O15A	-140.0
F14	C13	N15	O15B	39.7
N16	C13	N15	O15A	107.7
N16	C13	N15	O15B	-72.6
C12	C13	N16	O16A	59.8
C12	C13	N16	O16B	-115.4
F14	C13	N16	O16A	-177.7
F14	C13	N16	O16B	7.1
N15	C13	N16	O16A	-64.4
N15	C13	N16	O16B	120.4
C1	C2	C17	O18	44.6
C1	C2	C17	O19	-133.7
C3	C2	C17	O18	-68.1
C3	C2	C17	O19	113.6
C7	C2	C17	O18	166.0
C7	C2	C17	O19	-12.3
C2	C17	O19	C20	179.2
O18	C17	O19	C20	0.9
C17	O19	C20	C21	-171.6
O19	C20	C21	F22	59.3
O19	C20	C21	N23	-62.0
O19	C20	C21	N24	180.0
C20	C21	N23	O23A	-44.9
C20	C21	N23	O23B	135.5
F22	C21	N23	O23A	-170.0
F22	C21	N23	O23B	10.4
N24	C21	N23	O23A	74.7
N24	C21	N23	O23B	-104.9
C20	C21	N24	O24A	54.1
C20	C21	N24	O24B	-125.3
F22	C21	N24	O24A	178.1
F22	C21	N24	O24B	-1.2
N23	C21	N24	O24A	-67.6
N23	C21	N24	O24B	113.1